Mathematical Quantum Mechanics II

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Contents

Chapter 1

Principles of Quantum Mechanics

1.1 Hilbert spaces

Definition (Hilbert Spaces)**.** *A space $\mathscr{H}$ is a Hilbert space if*

- *$\mathscr{H}$ is a complex vector space;*
- *it is equipped with an inner product $\langle \cdot, \cdot \rangle$ which is linear in the second argument and anti-linear in the first*

$$\langle x, \lambda y \rangle = \lambda \langle x, y \rangle, \quad \langle \lambda x, y \rangle = \overline{\lambda} \langle x, y \rangle;$$

- *$(\mathscr{H}, \| \cdot \|)$ is a Banach (complete normed) space with norm $\|x\| = \sqrt{\langle x, x \rangle}$.*

A Hilbert space $\mathscr{H}$ is **separable** if there exists a finite or countable family of vectors $\{u_n\}_{n \geq 1}$ which forms an **orthonormal basis**. In this case, we can write

$$x = \sum_{n \geq 1} \langle u_n, x \rangle u_n, \quad \forall x \in \mathscr{H}.$$

Consequently, we have **Parsevel's identity**

$$\|x\|^2 = \sum_{n \geq 1} |\langle u_n, x \rangle|^2, \quad \forall x \in \mathscr{H}.$$

We will always work with separable Hilbert spaces.

Review: Riesz (representation)/Banach-Alaoglu/Banach-Steinhaus theorem.

1.2 Operators on Hilbert spaces

Definition (Operators on Hilbert Spaces)**.** *By an operator A on $\mathscr{H}$ we mean a linear map $A : D(A) \to \mathscr{H}$ with a dense, subspace $D(A)$ (domain of A).*
The **adjoint operator** *A^* is defined by*

$$D(A^*) = \Big\{ x \in \mathscr{H} \,|\, \exists\, A^*x \in \mathscr{H} : \langle x, Ay \rangle = \langle A^*x, y \rangle, \quad \forall y \in D(A) \Big\}.$$

The operator A is **self-adjoint** *if $A = A^*$.*

The concept of self-adjointness is very important in quantum mechanics. Mathematically, it enables various rigorous computations, thanks to the **Spectral theorem**.

Theorem (Spectral theorem)**.** *Assume that A is a self-adjoint operator on a separable Hilbert space $\mathscr{H}$. Then there exists a measure space (Ω, μ), a real-valued measurable function $a : \Omega \to \mathbb{R}$ and a unitary transformation $U : \mathscr{H} \to L^2(\Omega)$ such that*

$$UAU^* = M_a.$$

Here M_a is the **multiplication operator** *on $L^2(\Omega)$, defined by*

$$(M_a f)(x) = a(x)f(x), \quad D(M_a) = \{f \in L^2(\Omega), af \in L^2(\Omega)\}.$$

We can choose $\Omega = \sigma(A) \times \mathbb{N} \subset \mathbb{R}^2$ and $a(\lambda, n) = \lambda$.

In practice, the self-adjointness is not always easy to prove. It is however easier to check whenever an operator A is **symmetric**, namely

$$\langle x, Ay \rangle = \langle Ax, y \rangle, \quad \forall x, y \in D(A).$$

Exercise. *Prove that the followings are equivalent:*

1. *A is a symmetric operator;*
2. *$\langle x, Ax\rangle \in \mathbb{R}$ for all $x \in D(A)$.*
3. *A^* is an extension of A, namely $D(A) \subset D(A^*)$.*

Thus if A is self-adjoint, then A is symmetric. But the reverse is not true. Two useful methods to find **self-adjoint extensions** for symmetric operators are **Friedrichs' extension** and **Kato-Rellich theorem**.

Theorem (Friedrichs' extension)**.** *Assume that A is bounded from below, namely*

$$\langle x, Ax\rangle \geq -C\|x\|^2, \quad \forall x \in D(A)$$

with a finite constant C independent of x. Then A has a self-adjoint extension A_F by Friedrichs' method. The Friedrichs extension preserves the **ground state energy**

$$\inf_{x\in D(A), \|x\|=1} \langle x, Ax\rangle = \inf_{x \in D(A_F), \|x\|=1} \langle x, A_F x\rangle.$$

The **quadratic form domain** $Q(A_F)$ is the same with $Q(A)$. Recall that we define $Q(A)$ as the closure of $D(A)$ under the quadratic form norm $\|x\|_{Q(A)} = \sqrt{\langle x, (A+C+1)x\rangle}$. However, the domain $D(A_F)$ is often not known explicitly. For the latter issue, the Kato-Rellich theorem gives a better information on the domain of the extension.

Theorem (Kato-Rellich theorem)**.** *Assume that we can write $A = A_0 + B$, where A_0 is self-adjoint and B is a small perturbation of A_0, in the meaning that*

$$\|Bx\| \leq (1-\varepsilon)\|A_0 x\| + C_\varepsilon \|x\|, \quad \forall x \in D(A_0) \subset D(B),$$

for some constant $\varepsilon > 0$ independent of x (we say that B is A_0-relatively bounded with the relative bound $1-\varepsilon$). Then A can be extended to be a self-adjoint operator on the same domain of A_0.

Review: Bounded/compact/Hilbert-Schmidt/trace class operators.

1.3 Principles of Quantum Mechanics

Definition (Principles of Quantum Mechanics). *A quantum system can be described by a (separable) Hilbert space* $\mathscr{H}$*.*

- *A* **pure state** *is a rank-one projection* $|x\rangle\langle x|$ *with a normalized vector* $x \in \mathscr{H}$ *(we use the bra-ket notation). A* **mixed state** *is a trace class operator* Γ *on* $\mathscr{H}$ *such that* $\Gamma = \Gamma^* \geq 0$, $\operatorname{Tr}\Gamma = 1$*. By Spectral theorem any mixed state is a* **super-position** *of pure states, namely*

$$\Gamma = \sum_{n \geq 1} \xi_n |x_n\rangle\langle x_n|$$

  where $\{x_n\}$ *is an orthonormal family in* $\mathscr{H}$ *and* $\xi_n \geq 0$, $\sum_n \xi_n = 1$.

- *The* **Hamiltonian** H *is a self-adjoint operator on* $\mathscr{H}$ *which corresponds to the energy* $\langle x, Hx\rangle$ *or* $\operatorname{Tr}(H\Gamma)$*. The ground state energy is*

$$E_0 := \inf \sigma(H) = \inf_{\|x\|=1} \langle x, Hx\rangle = \inf_{\Gamma \geq 0, \operatorname{Tr}\Gamma = 1} \operatorname{Tr}(H\Gamma).$$

  If the infimum exists, then the **ground state** *solves the Schrödinger equation* $Hx = E_0 x$*. Other elements of the spectrum* $\sigma(H)$ *corresponds to* **excited states**.

- *At a positive temperature* $T > 0$*, the minimizer of the* **free energy**

$$E_T = \inf_{\Gamma \geq 0, \operatorname{Tr}\Gamma = 1} \Big\{ \operatorname{Tr}(H\Gamma) + T \operatorname{Tr}\Big(\Gamma \log(\Gamma)\Big) \Big\}$$

  is given uniquely by the **Gibbs state**

$$\Gamma_T = Z_T^{-1} e^{-H/T}, \quad Z_T = \operatorname{Tr}(e^{-H/T}) \quad \textit{(if the partition function } Z_T \textit{ is finite).}$$

- *The evolution of the quantum system is determined by the* **time-dependent Schrödinger equation** $x(t) = e^{-itH} x_0$.

Exercise. *Prove that if the infimum*

$$E_0 := \inf \sigma(H) = \inf_{\|x\|=1} \langle x, Hx \rangle = \inf_{\Gamma \geq 0, \operatorname{Tr}\Gamma = 1} \operatorname{Tr}(H\Gamma).$$

is attained for a mixed state Γ, then it is also attained for a pure state $|x\rangle\langle x|$.

Exercise. *Prove that any ground state $|x\rangle\langle x|$ satisfies the Schrödinger equation*

$$Hx = E_0 x.$$

Hint: For any $y \in \mathscr{H}$, define $x_\varepsilon = (x+\varepsilon y)/|x+\varepsilon y\|$. Then the functional $\varepsilon \mapsto \langle x_\varepsilon, Hx_\varepsilon \rangle$ has a local minimum at $\varepsilon = 0$.

Exercise. *Assume that the partition function is finite for some temperature $T_0 > 0$.*
1. Prove that Z_T it is finite for all $T \in (0, T_0)$. This implies that the Gibbs states is well-defined for all $T \in (0, T_0)$.
2. Prove that the free energy is finite for all $T \in (0, T_0)$ and

$$\lim_{T \to 0} E_T = E_0 \quad \textit{(the ground state energy).}$$

Hint: You can use the Gibbs variational principle $E_T = -T \log Z_T$.

1.4 Many-body quantum mechanics

Definition (Tensor product). *Let $\mathscr{H}_1$ and $\mathscr{H}_2$ are two Hilbert spaces. The* **tensor product space** $\mathscr{H}_1 \otimes \mathscr{H}_2$ *is a Hilbert space*

$$\mathscr{H}_1 \otimes \mathscr{H}_2 = \overline{\mathrm{Span}\{u \otimes v \,|\, u \in \mathscr{H}_1, v \in \mathscr{H}_2\}}.$$

Here the closure is taken under the norm of $\mathscr{H}_1 \otimes \mathscr{H}_2$ which is given by the inner product

$$\langle u_1 \otimes u_2, v_1 \otimes v_2 \rangle_{\mathscr{H}_1 \otimes \mathscr{H}_2} = \langle u_1, v_1 \rangle_{\mathscr{H}_1} \langle u_2, v_2 \rangle_{\mathscr{H}_2}.$$

Let A_1 and A_2 are operators on $\mathscr{H}_1$ and $\mathscr{H}_2$, respectively. Then the **tensor product operator** $A_1 \otimes A_2$ *is an operator on $\mathscr{H}_1 \otimes \mathscr{H}_2$ defined by*

$$A_1 \otimes A_2(u_1 \otimes u_2) = (A_1 u_1) \otimes (A_2 u_2), \quad D(A_1 \otimes A_2) = D(A_1) \otimes D(A_2).$$

More generally, we can define the tensor product space $\mathscr{H}_1 \otimes \mathscr{H}_2 \otimes ... \otimes \mathscr{H}_N$ and the tensor product operator $A_1 \otimes A_2 \otimes ... \otimes A_N$. In particular, if $\mathscr{H}_1 = \mathscr{H}_2 = ... = \mathscr{H}_N$, then we write

$$\mathscr{H}_1 \otimes \mathscr{H}_1 \otimes ... \otimes \mathscr{H}_1 = \mathscr{H}_1^{\otimes N}.$$

Remarks:

- The tensor product $\mathscr{H}_1 \otimes \mathscr{H}_2$ is **different** from the direct product $\mathscr{H}_1 \times \mathscr{H}_2$. In particular, for any $\lambda \in \mathbb{C}$ we have

$$(\lambda u_1) \otimes u_2 = \lambda(u_1 \otimes u_2) = u_1 \otimes (\lambda u_2)$$

  and similarly

$$(\lambda A_1) \otimes A_2 = \lambda(A_1 \otimes A_2) = A_1 \otimes (\lambda A_2).$$

- The notation $\mathscr{H}_1 \otimes \mathscr{H}_2 \otimes ... \otimes \mathscr{H}_N$ is consistent thanks to the **Associative Property**

$$(\mathscr{H}_1 \otimes \mathscr{H}_2) \otimes \mathscr{H}_3 = \mathscr{H}_1 \otimes (\mathscr{H}_2 \otimes \mathscr{H}_3).$$

  The same applies to the tensor product operator $A_1 \otimes A_2 \otimes ... \otimes A_N$.

Exercise. *Assume that* $\{u_n\}_{n\geq 1}$ *is an orthonornal basis for* $\mathscr{H}_1$ *and* $\{v_m\}_{m\geq 1}$ *is an orthonornal basis for* $\mathscr{H}_2$*. Prove that* $\{u_n \otimes v_m\}_{m,n\geq 1}$ *is an orthonornal basis for* $\mathscr{H}_1 \otimes \mathscr{H}_2$*.*

Exercise. *Let* $\mathscr{H}_1$ *and* $\mathscr{H}_2$ *be two Hilbert spaces. Assume that the sequence* $\{u_n\}_{n\geq 1}$ *is bounded in* $\mathscr{H}_1$ *and the sequence* $\{v_n\}_{n\geq 1}$ *converges weakly to* 0 *in* $\mathscr{H}_2$*. Prove that*

$$u_n \otimes v_n \rightharpoonup 0 \quad \text{weakly in } \mathscr{H}_1 \otimes \mathscr{H}_2.$$

Exercise. *Prove that for any* $d, N \geq 1$*, we have* $L^2(\mathbb{R}^{dN}) = L^2(\mathbb{R}^d)^{\otimes N}$*.*

Definition (Many body quantum systems)**.** *Consider a quantum system of* N *particles, where the* i*-th particle is described by the Hilbert space* $\mathscr{H}_i$ *and the Hamiltonian* h_i*. Moreover, assume that the interaction between the* i*-th and* j*-th particles is described by an operator* W_{ij} *on* $\mathscr{H}_i \otimes \mathscr{H}_j$*. Then the combined system of* N *particles is described by the* **interacting Hamiltionian**

$$H_N = \sum_{i=1}^N h_i + \sum_{1\leq i<j\leq N} W_{ij}.$$

acting on the **tensor product space** $\mathscr{H}_1 \otimes ... \otimes \mathscr{H}_N$*. Here to simplify the notation we identify* h_i *with* $\mathbb{1}_{\mathscr{H}_1} \otimes ... \otimes h_i \otimes ... \otimes \mathbb{1}_{\mathscr{H}_N}$ *(the identity* $\mathbb{1}$ *is put everywhere except the* i*-th position). The same applies to* W_{ij}*, for example* W_{12} *is identified to* $W_{12} \otimes \mathbb{1}_{\mathscr{H}_3} \otimes ... \otimes \mathbb{1}_{\mathscr{H}_N}$*.*

Remarks: The above expression is a bit formal as we did not specify the domain of relevant operators. In practice, we will consider the case where W_{ij} is relatively bounded with respect to $h_i + h_j$, with an arbitrary small relative bound. In this case, by the Kato-Rellich theorem the interacting Hamiltonian is **self-adjoint** on the same domain with the **non interacting Hamiltionian**

$$H_N^0 = h_1 + ... + h_N.$$

Exercise (Non-interacting Hamiltonian). *Assume that for any $i = 1, 2, ..., N$, the Hamiltonian h_i is self-adjoint on $\mathscr{H}_i$. Consider the N-particle system with the non-interacting Hamiltonian $H_N^0 = h_1 + ... + h_N$ on $\mathscr{H}_1 \otimes ... \otimes \mathscr{H}_N$.*
1. Prove that H_N^0 is self-adjoint with the domain

$$D(H_N^0) = \overline{D(h_1) \otimes D(h_2) \otimes ... \otimes D(h_N)}^{\|\cdot\|_{H_N^0}}.$$

Here the closure is taken with the operator norm $\|\Psi_N\|_{H_N^0} = \|\Psi_N\| + \|H_N^0 \Psi_N\|$.
2. Prove that the ground state energy of H_N^0 is

$$\inf \sigma(H_N^0) = \sum_{i=1}^N \inf \sigma(h_i) \quad \textit{(both sides can be } -\infty\textit{)}.$$

3. Prove that if u_i is a ground state of h_i, then $u_1 \otimes ... \otimes u_N$ is a ground state of H_N^0.

In practice, we will mostly consider **identical particles**. For instance, every electron in the universe has the same mass, electric charge and spin. To work with identical particles, we will always assume that the corresponding one-body operators h_i is the same for all i, and that the interaction operator W_{ij} is the same for all i and j (in particular, $W_{ij} = W_{ji}$). The notations h_i and W_{ij} are still useful to indicate which particles that the operators act. Then the N-body Hamiltonian

$$H_N = \sum_{i=1}^N h_i + \sum_{1 \le i < j \le N} W_{ij}.$$

leaves invariant two important subspaces of $\mathscr{H}^{\otimes N}$: the **symmetric subspace** and the **anti-symmetric subspace**, which correspond to the **Bose-Einstein statistics** and the **Fermi-Dirac statistics**.

Definition (Particle statistics). *Let $\mathscr{H}$ be the Hilbert space of one particle. For every permutation $\sigma \in S_N$, we define the permutation operator $U_\sigma : \mathscr{H}^{\otimes N} \to \mathscr{H}^{\otimes N}$ by*

$$U_\sigma(u_1 \otimes u_2 \otimes ... \otimes u_N) = u_{\sigma(1)} \otimes u_{\sigma(2)} \otimes ... \otimes u_{\sigma(N)}.$$

- *For N identical* **bosons**, *the corresponding Hilbert space $\mathscr{H}^{\otimes_s N}$ is the* **symmetric**

subspace *of* $\mathscr{H}^{\otimes N}$*, namely*

$$U_\sigma(\Psi_N) = \Psi_N, \quad \forall \Psi_N \in \mathscr{H}^{\otimes_s N}, \quad \forall \sigma \in S_N.$$

- *For* N *identical* **fermions***, the corresponding Hilbert space* $\mathscr{H}^{\otimes_a N}$ *is the* **anti-symmetric subspace** *of* $\mathscr{H}^{\otimes N}$*, namely*

$$U_\sigma(\Psi_N) = \text{sign}(\sigma)\Psi_N, \quad \forall \Psi_N \in \mathscr{H}^{\otimes_a N}, \quad \forall \sigma \in S_N.$$

The latter identity is called **Pauli's exclusion principle***.*

Exercise. *1. Prove that the operator* U_σ *defined as above is a unitary transformation.*
2. Prove that the operators

$$P_+ = (N!)^{-1} \sum_{\sigma \in S_N} U_\sigma, \quad P_- = (N!)^{-1} \sum_{\sigma \in S_N} \text{sign}(\sigma) U_\sigma$$

are orthogonal projections, namely $P_\pm = P_\pm^* = P_\pm^2$*.*
3. Prove that $\mathscr{H}^{\otimes_s N} = P_+(\mathscr{H}^{\otimes N})$ *and* $\mathscr{H}^{\otimes_a N} = P_-(\mathscr{H}^{\otimes N})$*.*

Exercise. *Assume that* $\{u_n\}_{n\geq 1}$ *is an orthonormal basis for* $\mathscr{H}$*. Prove that*

$$\{P_\pm(u_{i_1} \otimes u_{i_2} \otimes ... \otimes u_{i_N})\}_{i_1,...,i_N \geq 1}$$

is an orthogonal basis for $\mathscr{H}^{\otimes_{s/a} N}$*.*

The simplest example for a bosonic state is the **Hartree state** (pure tensor product state)

$$u^{\otimes N}(x_1, ..., x_N) = u(x_1)...u(x_N)$$

where u is a normalized vector in $\mathscr{H}$. The simplest example for a fermionic state is the **Slater determinant**

$$(u_1 \wedge u_2 \wedge ... \wedge u_N)(x_1, ..., x_N) = \frac{1}{\sqrt{N!}} \det \left[(u_i(x_j))_{1 \leq i,j \leq N} \right]$$

where $\{u_i\}_{i=1}^N$ is an orthonormal family of $\mathscr{H}$. Here we put the factor $1/\sqrt{N!}$ to ensure that the Slater determinant is normalized (you should check why?).

The behavior of a many-body quantum system depends crucially on the particle statistics. This can be seen already in the non-interacting case.

Exercise (Non-interacting Hamiltonian with particle statistics)**.** *Let h be a self-adjoint operator on $\mathscr{H}$. Consider the non-interacting Hamiltonian $H_N^0 = h_1 + ... + h_N$ on $\mathscr{H}^{\otimes_{a/s} N}$.*

1. Prove that H_N^0 is self-adjoint with the domain

$$D(H_N^0) = P_{\pm}\overline{D(h) \otimes D(h) \otimes ... \otimes D(h)}^{\|\cdot\|_{H_N^0}}.$$

2. Prove that in the bosonic case, the ground state energy of H_N^0 is

$$\inf \sigma(H_N^0) = N \inf \sigma(h) \quad \textit{(both sides can be } -\infty\textit{).}$$

In particular, if u is a ground state for h, then the Hartree state $u^{\otimes N}$ is a ground state for H_N^0.

*3. (**Hard**) Prove that in the fermionic case, the ground state energy of H_N^0 is*

$$\inf \sigma(H_N^0) = \sum_{i=1}^N \lambda_i(h) \quad \textit{(both sides can be } -\infty\textit{).}$$

Here λ_i is the i-th min-max value of h. In particular, if h has the lowest eigenvalues $\lambda_1, ..., \lambda_N$ with eigenfunctions $u_1, ..., u_N$, then the Slater determinant $u_1 \wedge u_2 \wedge ... \wedge u_N$ is a ground state for H_N^0.

In general, non-interacting systems are "easy to understand". The interacting systems are much more difficult. When the number of particles becomes large, basic physical properties of interacting systems are **impossible to compute, even numerically**. In computational physics (even chemistry) people often use approximate theories: it is desirable to replace the **linear, many-body** theory by **nonlinear, one-body** (or few-body) theories. A major task of mathematical physics is to develop/justify these approximations.

Since the underlying Hilbert spaces $\mathscr{H}^{\otimes_{s/a} N}$ are too large, it is often useful to restrict to smaller classes of quantum states. For bosons, by restricting the consideration to only Hartree states, we obtain the **Hartree theory** (also called the **Gross-Pitaevskii theory** in the context of the **Bose-Einstein condensate** and superfluidity). For fermions, by restricting the consideration to only Slater determinants, we obtain the **Hartree-Fock theory**. These theories are consistent with the **mean-field approximation** and typically predict the leading order behavior of many-body quantum systems when the number of particles becomes large.

To go beyond the leading order approximation, we need to take the **particle correlation** into account. The correction to the leading order approximation can be formulated in terms of **quasi-free particles**, leading to **Bogoliubov theory** for bosons, and the **Hartree-Fock-Bogoliubov theory** for fermions (the latter is a generalization of the **Bardeen-Cooper-Schrieffer theory** in the context of superconductivity).

In this course we will develop mathematical tools to derive rigorously these approximate theories. In particular, we will employ the framework from quantum field theory, including the **Fock space formalism** and the method of **second quantization**.

Chapter 2

Schrödinger operators

Definition. *A typical* **many-body Schrödinger operator** *has the form*

$$H_N = \sum_{i=1}^{N} (-\Delta_{x_i} + V(x_i)) + \sum_{1 \le i < j \le N} W(x_i - x_j)$$

acting on $L^2(\mathbb{R}^{dN})$ *or the bosonic space* $L^2(\mathbb{R}^d)^{\otimes_s N}$ *or the fermionic space* $L^2(\mathbb{R}^d)^{\otimes_a N}$*, where*

- $-\Delta$*, the usual Laplacian on* $L^2(\mathbb{R}^d)$*, is the* **kinetic operator** *of a particle;*
- $V : \mathbb{R}^d \to \mathbb{R}$ *an* **external potential***;*
- $W = W(-.) : \mathbb{R}^d \to \mathbb{R}$ *an* **interaction potential** *(it is even, hence* $W_{ij} = W_{ji}$*).*

Recall that the bosonic space $L^2(\mathbb{R}^d)^{\otimes_s N}$ contains all symmetric functions, namely

$$\Psi_N(x_1, ..., x_i, ..., x_j, ..., x_N) = \Psi_N(x_1, ..., x_j, ..., x_i, ..., x_N), \quad \forall i \neq j$$

while the fermionic space $L^2(\mathbb{R}^d)^{\otimes_a N}$ contains all anti-symmetric functions

$$\Psi_N(x_1, ..., x_i, ..., x_j, ..., x_N) = -\Psi_N(x_1, ..., x_j, ..., x_i, ..., x_N), \quad \forall i \neq j.$$

In this chapter the particle statistics does not play an important role, so at first reading you may think of H_N acting on the full space $L^2(\mathbb{R}^{dN})$ for simplicity.

We will study some general spectral properties of the Schrödinger operators. We will always assume that the interaction potential W is relatively bounded with respect to $-\Delta_{\mathbb{R}^d}$. For the external potential, we distinguish two different cases:

- The trapping case $V(x) \to +\infty$ as $|x| \to \infty$;
- The vanishing case $V(x) \to 0$ as $|x| \to \infty$.

The spectral properties of these two cases are very different. In the first case, the Hamiltonian H_N has discrete spectrum with eigenvalues converging to infinity. This follows the same analysis that we have discussed in MQM1 (we will recall below). In the second case, the interaction operator is **not a compact-perturbation** of the kinetic operator, leading to a big change on the essential spectrum in comparison to the one-body Schrödinger operator.

2.1 Weyl's theory

Let us quickly remind some important tools to study the Schrödinger operators. First we recall some general facts from spectral theory.

Definition (Spectrum)**.** *Let A be a self-adjoint operator on a Hilbert space $\mathscr{H}$. Then its spectrum is*

$$\sigma(A) = \{\lambda \in \mathbb{R} : (A-\lambda)^{-1} \textit{ is a bounded operator } \}.$$

The **discrete spectrum** $\sigma_{\text{dis}}(A)$ *is the set of isolated eigenvalues with finite multiplicities. The* **essential spectrum** *is the complement*

$$\sigma_{\text{ess}}(A) = \sigma(A) \backslash \sigma_{\text{dis}}(A).$$

Exercise. *Consider the multiplication operator M_a on $L^2(\Omega, \mu)$ which is self-adjoint with the domain $D(M_a) = \{f \in L^2 : af \in L^2\}$. Prove that*

- $\lambda \in \sigma(M_a)$ *iff* $\mu(a^{-1}(\lambda-\varepsilon, \lambda+\varepsilon)) > 0$ *for all* $\varepsilon > 0$, *namely* $\sigma(M_a) = \text{ess-range}(a)$.
- λ *is an eigenvalue of* M_a *iff* $\mu(a^{-1}(\lambda)) > 0$.
- $\lambda \in \sigma_{\text{dis}}(M_a)$ *iff* λ *is an isolated point of* $\sigma(M_a)$ *and* $0 < \mu(a^{-1}(\lambda)) < \infty$.

By the spectral theorem, any self-adjoint operator is unitarily equivalent to a multiplication operator. However, this abstract result is not very helpful in application, as it is hard to compute the measure μ.

Here is a general characterization of the spectrum.

Theorem (Weyl's Criterion). *For any self-adjoint operator A on a Hilbert space $\mathscr{H}$:*

- $\lambda \in \sigma(A)$ *iff there exists a* **Weyl sequence** $\{u_n\} \subset D(A)$ *such that*

$$\|u_n\| = 1, \quad \|(A-\lambda)u_n\| \to 0 \quad as \quad n \to \infty.$$

- $\lambda \in \sigma_{\text{ess}}(A)$ *iff there exists a Weyl sequence* $\{x_n\} \subset D(A)$ *such that*

$$\|u_n\| = 1, \quad u_n \rightharpoonup 0 \text{ **weakly,**} \quad \|(A-\lambda)u_n\| \to 0 \quad as \quad n \to \infty.$$

In practice, Weyl's Criterion is very useful to study the essential spectrum. A famous consequence of Weyl's Criterion is

Theorem (Compact perturbation does not change essential spectrum). *Let A be a self-adjoint operator on a Hilbert space. Let B be a symmetric operator which is A-relatively compact, namely $D(B) \subset D(A)$ and $B(A+i)^{-1}$ is a compact operator. Then $A+B$ is self-adjoint on $D(A)$ and*

$$\sigma_{\text{ess}}(A+B) = \sigma_{\text{ess}}(A).$$

Exercise. *Prove the above corollary using Weyl's Criterion theorem.*
Hint: You can write $B = B(A+i)^{-1}(A+i)$.

2.2 Min-max principle

A useful tool to study the discrete spectrum below the essential spectrum is the min-max principle.

Theorem (Min-Max Principle). *Let A be a self-adjoint operator on a Hilbert space $\mathscr{H}$.*

Assume that A is bounded from below and define the **min-max values**

$$\mu_n(A) = \inf_{\substack{M \subset D(A) \\ \dim M = n}} \sup_{\substack{u \in M \\ \|u\|=1}} \langle u, Au \rangle .$$

Then we have

$$\inf \sigma_{\text{ess}}(A) = \mu_\infty(A) := \lim_{n \to \infty} \mu_n(A).$$

Moreover, if $\mu_n(A) < \mu_\infty(A)$, then $\mu_1, \ldots, \mu_n$ are the lowest eigenvalues of A.

Remarks:

- In the above definition, the condition $M \subset D(A)$ can be replaced by $M \subset \mathfrak{D}$ for any subspace $\mathfrak{D}$ which is dense in the quadratic form domain $Q(A)$. Thus in practice, we can compute the min-max values even if we do not know the domain of A. For example, if A is the Friedrichs' extension of a (densely defined) operator A_0, then the min-max values can be computed using the domain of A_0.

- It is obvious that $\mu_n(A)$ is an increasing sequence when n grows. Thus the limit $\mu_\infty(A) := \lim_{n\to\infty} \mu_n(A)$ always exists, even it can be $+\infty$.

- If $\mu_\infty(A) = +\infty$, then the strict inequality $\mu_n(A) < \mu_\infty(A)$ trivially holds for all $n = 1, 2, ...$ Consequently, all min-max values become eigenvalues and they converge to $+\infty$. In this case we say that A has **compact resolvent** because $(A + C)^{-1}$ is a compact operator for any $C > -\mu_1(A)$).

- The min-max values is **monotone increasing in operator**, namely if $A \leq B$, then

  $$\mu_n(A) \leq \mu_n(B), \quad \forall n = 1, 2, ...$$

  In particular, if $A \leq B$ and A has compact resolvent, then B has compact resolvent.

2.3 Sobolev inequalities

Next, we turn to the fact that the Schrödinger operators are defined on the real space $\mathbb{R}^{dN}$. Therefore, we recall some standard results from real analysis.

Definition (Sobolev Spaces)**.** *For any dimension $d \geq 1$ and $s > 0$, define*

$$H^s(\mathbb{R}^d) := \Big\{ f \in L^2(\mathbb{R}^d) \,\Big|\, |k|^s \widehat{f}(k) \in L^2(\mathbb{R}^d) \Big\}$$

with $\hat{f}$ the Fourier transform of f. This is a Hilbert space with the inner product

$$\langle f, g \rangle_{H^s} = \int\limits_{\mathbb{R}^d} \overline{\widehat{f}(k)} \widehat{g}(k)(1 + |2\pi k|^2)^s \mathrm{d}k$$

Remarks:

- We use the following convention of the Fourier transform

$$\widehat{f}(k) = \int_{\mathbb{R}^d} e^{-2\pi i k \cdot x} f(x) dx.$$

- On the Sobolev space $H^s(\mathbb{R}^d)$, we can define the weak derivative via the Fourier transform

$$\widehat{D^\alpha f}(k) = (-2\pi i k)^\alpha \widehat{f}(k)$$

  which belongs to $L^2(\mathbb{R}^d)$ for any multiple index $\alpha = (\alpha_1, ..., \alpha_d)$ with $|\alpha| = \alpha_1 + ... + \alpha_d \leq s$.

- In the above definition and the Sobolev inequalities below, the power s is not necessarily an integer. In the course we will mostly think of s as an integer for simplicity. The non-integer case (the so-called **fractional Sobolev spaces**) is useful for studying relativistic quantum mechanics.

Theorem (Sobolev Inequalities/Continuous embedding)**.** *Let $d \geq 1$ and $s > 0$. Then*

$$\|f\|_{L^p(\mathbb{R}^d)} \leq C \|f\|_{H^s(\mathbb{R}^d)}, \quad \forall f \in H^s(\mathbb{R}^d)$$

where

$$\begin{cases} 2 \leqslant p \leqslant \frac{2d}{d-2s}, & \text{if } s < d/2, \\ 2 \leqslant p < \infty, & \text{if } s = d/2 \\ 2 \leqslant p \leqslant \infty, & \text{if } s > d/2. \end{cases}$$

We say that $H^s(\mathbb{R}^d) \subset L^p(\mathbb{R}^d)$ with continuous embedding. When $s > d/2$ we also have the continuous embedding $H^s(\mathbb{R}^d) \subset \mathscr{C}(\mathbb{R}^d)$ (the space of continuous functions with sup-norm).

Remarks:

- In the case $s < d/2$, the power $p^* := 2d/(d-2s)$ is called the **Sobolev critical exponent**. In fact, this is the **only power** works for the following standard Sobolev inequality
$$\|f\|_{L^{p^*}(\mathbb{R}^d)} \le C\|(-\Delta)^{s/2} f\|_{L^2(\mathbb{R}^d)}$$
(on the right side we do not put the full norm of H^s, but only the seminorm of $\dot{H}^s$).

- In principle, for any given power $s > 0$, the Sobolev inequality becomes weaker when the dimension d grows. For example,
$$H^1(\mathbb{R}) \subset L^2(\mathbb{R}) \cap \mathscr{C}(\mathbb{R}), \quad H^1(\mathbb{R}^2) \subset \bigcap_{2\le p<\infty} L^p(\mathbb{R}^2), \quad H^1(\mathbb{R}^3) \subset \bigcap_{2\le p\le 6} L^p(\mathbb{R}^2).$$
Similarly,
$$H^2(\mathbb{R}^3) \subset L^2(\mathbb{R}^3) \cap \mathscr{C}(\mathbb{R}^3) \quad \text{but} \quad H^2(\mathbb{R}^4) \not\subset \mathscr{C}(\mathbb{R}^4).$$

- A common difficulty of many-body quantum mechanics is that we will often work on spaces with very high dimensions, making the use of Sobolev inequality less efficient.

Theorem (Sobolev compact embedding). *Let $d \ge 1$ and $s > 0$. Then for any bounded set $\Omega \subset \mathbb{R}^d$, the operator $\mathbb{1}_\Omega : H^s(\mathbb{R}^d) \to L^p(\mathbb{R}^d)$ is a compact operator, where*
$$\begin{cases} 2 \leqslant p < \frac{2d}{d-2s}, & \text{if } s \le d/2, \\ 2 \leqslant p \leqslant \infty, & \text{if } s > d/2. \end{cases}$$
When $s > d/2$, we also have the compact embedding $\mathbb{1}_\Omega : H^s(\mathbb{R}^d) \to \mathscr{C}(\mathbb{R}^d)$.

Remark: An easy way to remember the Sobolev compact embedding is that if $u_n \rightharpoonup 0$ weakly in **any Sobolev space** $H^s(\mathbb{R}^d)$ with $s > 0$, then for any $R > 0$ we have
$$\|u_n \mathbb{1}(|x| \le R)\|_{L^2(\mathbb{R}^d)} \to 0.$$

Then the strong convergence in L^p follows by a standard interpolation (Hölder inequality); this is the reason we have to avoid the critical power (end-point).

Exercise. *Assume that $u_n \rightharpoonup 0$ weakly in a Sobolev space $H^s(\mathbb{R}^d)$ with $s > 0$. Prove that up to a subsequence $n \to \infty$, we can choose $R_n \to \infty$ such that*

$$\|u_n \mathbb{1}(|x| \le R_n)\|_{L^2(\mathbb{R}^d)} \to 0.$$

Is it really necessary to take a subsequence?

2.4 IMS formula

Another helpful result from real analysis is the **IMS formula**, named after **I**smagilov, **M**organ, **S**imon and **I**srael **M**ichael **S**igal. This provides with a **localization technique** in the position/configuration space.

Theorem (IMS formula)**.** *For any smooth function $\varphi : \mathbb{R}^d \to \mathbb{R}$ (e.g. $\mathscr{C}^1$ or Lipschitz), we have*

$$\frac{\varphi^2(-\Delta_{\mathbb{R}^d}) + (-\Delta_{\mathbb{R}^d})\varphi^2}{2} = \varphi(-\Delta_{\mathbb{R}^d})\varphi - |\nabla\varphi|^2.$$

Consequently, if smooth functions $\{\varphi_j\}_{j=1}^k$ form a **partition of unity**,

$$\sum_{j=1}^k |\varphi_j|^2 = \mathbb{1}_{\mathbb{R}^d},$$

then

$$-\Delta_{\mathbb{R}^d} = \sum_{j=1}^k \varphi_j(-\Delta_{\mathbb{R}^d})\varphi_j - \sum_{j=1}^k |\nabla\varphi_j|^2.$$

Exercise. *Prove the IMS formula using the integration by part.*

2.5 Schrödinger operators with trapping potentials

Theorem. *Consider the Schrödinger operator*

$$H_N = \sum_{i=1}^{N}(-\Delta_{x_i} + V(x_i)) + \sum_{1\le i<j\le N} W(x_i - x_j)$$

acting on $L^2(\mathbb{R}^{dN})$ *or* $L^2(\mathbb{R}^d)^{\otimes_s N}$ *or* $L^2(\mathbb{R}^d)^{\otimes_a N}$*. Assume that*

- $W \in L^p(\mathbb{R}^d) + L^\infty(\mathbb{R}^d)$ *with* $p > \max(d/2, 1)$
- $V \in L^p_{\text{loc}}(\mathbb{R}^d)$ *and* $V(x) \to +\infty$ *as* $|x| \to \infty$.

Then H_N*, originally defined on the core domain of smooth functions with compact support, is bounded from below and can be extended to be a self-adjoint operator by Friedrichs method. Moreover,* H_N *has compact resolvent, namely it has* **discrete spectrum with eigenvalues converging to** $+\infty$*.*

Proof. **Step 1.** We prove that H_N is bounded from below.

Consider the external potential $V : \mathbb{R}^d \to \mathbb{R}$. For any $\varepsilon > 0$ we can write

$$V = V_1 + V_2, \quad \|V_1\|_{L^p(\mathbb{R}^d)} \le \varepsilon, \quad V_2 \ge -C_\varepsilon, \quad \lim_{|x|\to\infty} V_2(x) = +\infty.$$

Consider a wave function $\Psi_N \in C_c^\infty(\mathbb{R}^{dN})$ (or a symmetric/anti-symmetric one) by Holder's inequality we have

$$\langle \Psi_N, V_1(x_1)\Psi_N\rangle = \int_{\mathbb{R}^{dN}} V_1(x_1)|\Psi_N(x_1,...,x_N)|^2 \mathrm{d}x_1...\mathrm{d}x_N$$
$$\ge -\int_{\mathbb{R}^{d(N-1)}} \Big(\int_{\mathbb{R}^d} |V_1(x_1)|^p \mathrm{d}x_1\Big)^{1/p}\Big(\int_{\mathbb{R}^d} |\Psi_N(x_1,...,x_N)|^{2q}\mathrm{d}x_1\Big)^{1/q}\mathrm{d}x_2...\mathrm{d}x_N$$

with

$$\frac{1}{p} + \frac{1}{q} = 1.$$

Here we have

$$\Big(\int_{\mathbb{R}^d} |V_1(x_1)|^p dx_1\Big)^{1/p} = \|V_1\|_{L^p(\mathbb{R}^d)} \le \varepsilon.$$

The condition $p > \max(1, d/2)$ implies that $q < \infty$ for all $d \ge 1$, and moreover $q < 2d/(d-2)$

in case $d \geq 3$. Thus by Sobolev's inequality for $H^1(\mathbb{R}^d)$,

$$\Big(\int_{\mathbb{R}^d} |\Psi_N(x_1,...,x_N)|^{2q} \mathrm{d}x_1\Big)^{1/q} \leq \int_{\mathbb{R}^d} |(1-\Delta_{x_1})^{1/2}\Psi_N|^2 \mathrm{d}x_1.$$

In summary,

$$\langle \Psi_N, V_1(x_1)\Psi_N\rangle \geq -C\varepsilon \int_{\mathbb{R}^{d(N-1)}} \Big(\int_{\mathbb{R}^d} |(1-\Delta_{x_1})^{1/2}\Psi_N|^2 \mathrm{d}x_1\Big) \mathrm{d}x_2...\mathrm{d}x_N = -C\varepsilon\langle \Psi_N, (1-\Delta_{x_1})\Psi_N\rangle.$$

This bound can be written in the compact form

$$V_1(x_1) \geq -C\varepsilon(1-\Delta_{x_1}).$$

Similar estimates holds for $V_1(x_2),...,V_1(x_N)$. Thus

$$\sum_{i=1}^N V(x_i) = \sum_{i=1}^N V_1(x_i) + \sum_{i=1}^N V_2(x_i) \geq \sum_{i=1}^N V_2(x_i) - C\varepsilon\sum_{i=1}^N (\Delta_{x_i}) - C_{\varepsilon,N}.$$

Consider the interaction potential $W : \mathbb{R}^d \to \mathbb{R}$. For any $\varepsilon > 0$ we can write

$$W = W_1 + W_2, \quad \|W_1\|_{L^p(\mathbb{R}^d)} \leq \varepsilon, \quad \|W_2\|_{L^\infty} \leq C_\varepsilon$$

Similarly as above, for any wave function $\Psi_N \in C_c^\infty(\mathbb{R}^{dN})$ (or a symmetric/anti-symmetric one) by Holder's inequality and Sobolev inequality we can bound

$$\begin{aligned}
&\langle \Psi_N, W_1(x_1-x_2)\Psi_N\rangle = \int_{\mathbb{R}^{dN}} W_1(x_1-x_2)|\Psi_N(x_1,...,x_N)|^2 \mathrm{d}x_1...\mathrm{d}x_N \\
&\geq -\int_{\mathbb{R}^{d(N-1)}} \Big(\int_{\mathbb{R}^d} |W_1(x_1-x_2)|^p \mathrm{d}x_1\Big)^{1/p}\Big(\int_{\mathbb{R}^d} |\Psi_N(x_1,...,x_N)|^{2q}\mathrm{d}x_1\Big)^{1/q} \mathrm{d}x_2...\mathrm{d}x_N \\
&\geq -\int_{\mathbb{R}^{d(N-1)}} \|W_1\|_{L^p(\mathbb{R}^d)}\Big(C\int_{\mathbb{R}^d} |(1-\Delta_{x_1})^{1/2}\Psi_N|^2\mathrm{d}x_1\Big)\mathrm{d}x_2...\mathrm{d}x_N \\
&\geq -C\varepsilon\langle \Psi_N, (1-\Delta_{x_1})\Psi_N\rangle.
\end{aligned}$$

Here again we use the notation $\frac{1}{p}+\frac{1}{q}=1$ and the condition $q<\infty$, $q<2d/(d-2)$ for $d \geq 3$. The only difference to the previous treatment of the external potential is that we use the **translation-invariance** of the interaction potential and the Lebesgue measure which ensure that

$$\Big(\int_{\mathbb{R}^d} |W_1(x_1-x_2)|^p \mathrm{d}x_1\Big)^{1/p} = \|W_1\|_{L^p(\mathbb{R}^d)} \leq \varepsilon.$$

The above estimate also holds for $W_1(x_i - x_j)$ for any $i \neq j$. Thus

$$\begin{aligned}\sum_{1\le i<j\le N} \langle \Psi_N, W_1(x_i-x_j)\Psi_N\rangle &\ge -C\varepsilon \sum_{1\le i<j\le N} \langle \Psi_N, (1-\Delta_{x_i})\Psi_N\rangle \\ &\ge -CN\varepsilon \sum_{i=1}^N \langle \Psi_N, (-\Delta_{x_i})\Psi_N\rangle - C_{\varepsilon,N}.\end{aligned}$$

The potential W_2 is bounded, and hence for the total interaction part, we have

$$\sum_{1\le i<j\le N} \langle \Psi_N, W(x_i-x_j)\Psi_N\rangle \ge -CN\varepsilon \sum_{i=1}^N \langle \Psi_N, (-\Delta_{x_i})\Psi_N\rangle - C_{\varepsilon,N}.$$

Conclusion of the lower bound. Combining the above estimates for the external and interaction potentials we conclude that

$$\sum_{i=1}^N V(x_i)) + \sum_{1\le i<j\le N} W(x_i-x_j) \ge \sum_{i=1}^N V_2(x_i) - C(N+1)\varepsilon \sum_{i=1}^N (-\Delta_{x_i}) - C_{\varepsilon,N}.$$

This holds for any $\varepsilon \in (0,1)$. We can choose $\varepsilon = \varepsilon_N > 0$ small enough such that $C(N+1)\varepsilon < 1/2$. Thus

$$H_N = \sum_{i=1}^N (-\Delta_{x_i} + V(x_i)) + \sum_{1\le i<j\le N} W(x_i-x_j) \ge \sum_{i=1}^N \Big(-\frac{1}{2}\Delta_{x_i} + V_2(x_i)\Big) - C_N.$$

Since V_2 is bounded from below, we conclude that H_N is bounded from below.

Consequently, H_N can be extended to be a self-adjoint operator using Friedrichs' method.

Step 2. We need to prove that H_N has compact resolvent. From the above lower bound

$$H_N \ge \sum_{i=1}^N \Big(-\frac{1}{2}\Delta_{x_i} + V_2(x_i)\Big) - C_N.$$

and the Min-max principle, it suffices to prove that the operator

$$\widetilde{H}_N = \sum_{i=1}^N \Big(-\frac{1}{2}\Delta_{x_i} + V_2(x_i)\Big)$$

has compact resolvent. This operator can be written as

$$\widetilde{H}_N = -\frac{1}{2}\Delta_{\mathbb{R}^{dN}} + U(X), \quad U(X) = \sum_{i=1}^{N} V_2(x_i), \quad X = (x_1, ..., x_N) \in \mathbb{R}^{dN}.$$

If H_N is an operator on the full space $L^2(\mathbb{R}^{dN})$, then we can interpret $\widetilde{H}_N$ as a **one-body Schrödinger operator on** $L^2(\mathbb{R}^{dN})$. The condition $\lim_{|x|\to\infty} V_2(x) \to +\infty$ implies that

$$\lim_{|X|\to\infty} U(X) = +\infty.$$

Therefore, $-\frac{1}{2}\Delta_{\mathbb{R}^{dN}} + U(X)$ has compact resolvent (we have proved this in MQM1). Consequently, the original operator H_N has compact resolvent.
Now consider the case when H_N is an operator on the bosonic space. Then by the definition, the min-max value of H_N is

$$\mu_n(H_N) = \inf_{\dim M = n} \sup_{\substack{u\in M \\ \|u\|=1}} \langle \Psi_N, H_N \Psi_N \rangle .$$

Here the infimum is taken over all symmetric subspaces M of $C_c^\infty(\mathbb{R}^{dN})$. The infimum does not increase if we ignore the symmetry condition on M, namely the min-max values of the bosonic Hamiltonian H_N are bigger than or equal to those of the Hamiltonian on the full space $L^2(\mathbb{R}^{dN})$. Thus the bosonic operator H_N has compact resolvent. Similarly, the fermionic operator H_N also has compact resolvent. *q.e.d.*

2.6 Schrödinger operators with vanishing potentials

Now we turn to the case when the external potential vanishes at infinity. A motivating example is the **Atomic Hamiltonian** with the Coulomb potentials $W(x) = |x|^{-1}$ and $V(x) = -Z|x|^{-1}$, $x \in \mathbb{R}^3$.

We start with the self-adjointness of the many-body Hamiltonian for general potentials.

Theorem (Kato theorem)**.** *Consider the Schrödinger operator*

$$H_N = \sum_{i=1}^{N}(-\Delta_{x_i} + V(x_i)) + \sum_{1\le i<j\le N} W(x_i - x_j)$$

acting on $L^2(\mathbb{R}^{dN})$ *or* $L^2(\mathbb{R}^d)^{\otimes_s N}$ *or* $L^2(\mathbb{R}^d)^{\otimes_a N}$. *Assume that*

$$W, V \in L^p(\mathbb{R}^d) + L^\infty(\mathbb{R}^d), \quad p > \max(d/2, 1)$$

Then H_N *is self-adjoint operator with the quadratic form domain*

$$Q(H_N) = H^1(\mathbb{R}^{dN}) \quad \textit{or } H^1_s(\mathbb{R}^{dN}) = P_+ H^1(\mathbb{R}^{dN}) \quad \textit{or } H^1_a(\mathbb{R}^{dN}) = P_- H^1(\mathbb{R}^{dN}).$$

Moreover, if we assume that

$$W, V \in L^p(\mathbb{R}^d) + L^\infty(\mathbb{R}^d), \quad p > \max(d/2, 2)$$

then the domain of H_N *is*

$$D(H_N) = H^2(\mathbb{R}^{dN}) \quad \textit{or } H^2_s(\mathbb{R}^{dN}) = P_+ H^2(\mathbb{R}^{dN}) \quad \textit{or } H^2_a(\mathbb{R}^{3N}) = P_- H^2(\mathbb{R}^{dN}).$$

Proof. **Part 1.** Consider the case $W, V \in L^p(\mathbb{R}^d) + L^\infty(\mathbb{R}^d), p > \max(d/2, 1)$. Proceeding exactly as in the case of trapping external potentials (now we just do not have $V_2(x) \to \infty$ as $|x| \to \infty$), then we obtain the lower bound

$$H_N \ge \frac{1}{2} \sum_{i=1}^N -\Delta_{x_i} - C_N.$$

Thus H_N is bounded from below. Consequently, it can be extended to be a self-adjoint operator by Friedichs' method.

Moreover, by the same argument we also get the upper bound

$$H_N \le 2 \sum_{i=1}^N -\Delta_{x_i} + C_N.$$

Thus the quadratic form domain of H_N is the same with the non-interacting Hamiltonian

$$\sum_{i=1}^N -\Delta_{x_i} = -\Delta_{\mathbb{R}^{dN}},$$

namely

$$Q(H_N) = H^1(\mathbb{R}^{dN}) \quad \text{or } H^1_s(\mathbb{R}^{dN}) = P_+ H^1(\mathbb{R}^{dN}) \quad \text{or } H^1_a(\mathbb{R}^{dN}) = P_- H^1(\mathbb{R}^{dN}).$$

Part 2. Consider the case $W, V \in L^p(\mathbb{R}^d) + L^\infty(\mathbb{R}^d), p > \max(d/2, 2)$. We can prove that the external and interaction potentials are relatively bounded with respect to the kinetic operator.

Let us consider the interaction potential $W : \mathbb{R}^d \to \mathbb{R}$. For any $\varepsilon > 0$ we can write

$$W = W_1 + W_2, \quad \|W_1\|_{L^p(\mathbb{R}^d)} \le \varepsilon, \quad \|W_2\|_{L^\infty} \le C_\varepsilon.$$

For any wave function Ψ_N by Hölder and Sobolev inequalities (for $H^2(\mathbb{R}^d)$) we can bound

$$\begin{aligned}
&\|W_1(x_1 - x_2)\Psi_N\|^2 = \int_{\mathbb{R}^{dN}} |W_1(x_1 - x_2)|^2 |\Psi_N(x_1, ..., x_N)|^2 \mathrm{d}x_1 ... \mathrm{d}x_N \\
&\le \int_{\mathbb{R}^{d(N-1)}} \Big(\int_{\mathbb{R}^d} |W_1(x_1 - x_2)|^p \mathrm{d}x_1 \Big)^{2/p} \Big(\int_{\mathbb{R}^d} |\Psi_N(x_1, ..., x_N)|^q \mathrm{d}x_1 \Big)^{2/q} \mathrm{d}x_2 ... \mathrm{d}x_N \\
&\le \int_{\mathbb{R}^{d(N-1)}} \|W_1\|^2_{L^p(\mathbb{R}^d)} \Big(C \int_{\mathbb{R}^d} |(1 - \Delta_{x_1})\Psi_N|^2 \mathrm{d}x_1 \Big) \mathrm{d}x_2 ... \mathrm{d}x_N \\
&\le C\varepsilon^2 \|(1 - \Delta_{x_1})\Psi_N\|^2.
\end{aligned}$$

Here we use the the notation

$$\frac{2}{p} + \frac{2}{q} = 1.$$

The condition $p > \max(d/2, 2)$ implies that $q < \infty$ for all $d \ge 1$, and moreover $q < 2d/(d-4)$ if $d > 4$, allowing to use the Sobolev inequality. The above estimate also holds for $W_1(x_i - x_j)$ for any $i \ne j$. Thus

$$\sum_{1 \le i < j \le N} \|W_1(x_i - x_j)\Psi_N\| \le C\varepsilon \sum_{1 \le i < j \le N} \|(1 - \Delta_{x_i})\Psi_N\| \le C\varepsilon N^2 \| \sum_{i=1}^N (-\Delta_{x_i})\Psi_N\| + C_{\varepsilon,N}.$$

In the latter estimate we also used that the non-negative operators $(-\Delta_{x_1})$, ..., $(-\Delta_{x_N})$ commute. Since W_2 is bounded, by the triangle inequality we conclude that

$$\Big\| \sum_{1 \le i < j \le N} W(x_i - x_j)\Psi_N \Big\| \le C\varepsilon N^2 \| \sum_{i=1}^N (-\Delta_{x_i})\Psi_N\| + C_{\varepsilon,N}.$$

The external potential can be treated similarly. Thus can choose $\varepsilon = \varepsilon_N > 0$ small enough such that

$$\Big\| \Big(\sum_{i=1}^N V(x_i) + \sum_{1 \le i < j \le N} W(x_i - x_j) \Big) \Psi_N \| \le \frac{1}{2} \| \sum_{i=1}^N (-\Delta_{x_i})\Psi_N\| + C_N.$$

By the Kato-Rellich theorem, we conclude that H_N is a self-adjoint operator on the same domain of

$$\sum_{i=1}^{N}(-\Delta_{x_i}) = -\Delta_{\mathbb{R}^{dN}},$$

namely

$$D(H_N) = H^2(\mathbb{R}^{dN}) \quad \text{or } H_s^2(\mathbb{R}^{dN}) = P_+ H^2(\mathbb{R}^{dN}) \quad \text{or } H_a^2(\mathbb{R}^{3N}) = P_- H^2(\mathbb{R}^{dN}).$$

q.e.d.

Remarks:

- For the atomic Hamiltonian, the Coulomb potential can be written as

$$|x|^{-1} = |x|^{-1}\mathbb{1}(|x| \le 1) + |x|^{-1}\mathbb{1}(|x| \ge 1) \in L^{3-\varepsilon}(\mathbb{R}^3) + L^{3+\varepsilon}(\mathbb{R}^3), \quad \forall \varepsilon > 0.$$

  Thus the condition $L^p + L^\infty$ in the above Theorem is clearly satisfied.

- For Coulomb potential, instead of using Sobolev inequality you may also use **Hardy's inequality**

$$-\Delta \ge \frac{1}{4|x|^2} \quad \text{on} \quad L^2(\mathbb{R}^3).$$

- The self-adjointness of the Atomic Hamiltonian was first proved by Kato in 1951. There is a nice story behind his proof; see "Tosio Kato's Work on Non-Relativistic Quantum Mechanics" by Barry Simon `https://arxiv.org/pdf/1711.00528.pdf`.

2.7 HVZ theorem

Unlike the case of trapping external potentials, the Hamiltonian with a vanishing external potential has continuous spectrum. If the **interaction potential is positive**, the essential spectrum was determined by Huntiker, Van Winter and Zhislin in 1960s.

Theorem (HVZ theorem)**.** *Consider the Schrödinger operator*

$$H_N = \sum_{i=1}^{N}(-\Delta_{x_i} + V(x_i)) + \sum_{1 \le i < j \le N} W(x_i - x_j)$$

acting on $L^2(\mathbb{R}^{dN})$ *or* $L^2(\mathbb{R}^d)^{\otimes_s N}$ *or* $L^2(\mathbb{R}^d)^{\otimes_a N}$. *Assume that* $W \geq 0$ *and*

$$W, V \in L^p(\mathbb{R}^d) + L^q(\mathbb{R}^d), \quad \infty > p, q > \max(d/2, 2).$$

Then

$$\sigma_{\text{ess}}(H_N) = [E_{N-1}, \infty), \quad E_{N-1} = \inf \sigma(H_{N-1}).$$

Remarks:

- The condition $W \geq 0$ is needed for the inclusion $\sigma_{\text{ess}}(H_N) \subset [E_{N-1}, \infty)$. The inclusion $[E_{N-1}, \infty) \subset \sigma_{\text{ess}}(H_N)$ always holds true without the condition $W \geq 0$.
- For the one-body operator $-\Delta + U(x)$ on $\mathbb{R}^d$, if U vanishes at infinity, then it is a compact perturbation of the free Schrodinger operator $-\Delta$. Therefore, by Weyl's theorem, we know that

  $$\sigma_{\text{ess}}(-\Delta + U) = \sigma(-\Delta) = [0, \infty).$$

  The picture changes completely for the many-body Hamiltonian H_N. The reason is that the interaction $W(x_i - x_j)$ **does not vanish at infinity** even if the function $W : \mathbb{R}^d \to \mathbb{R}$ vanishes at infinity (because x_i and x_j may converge to infinity while their distance remains bounded).
- The difference $E_N - E_{N-1}$ (so called **binding energy**) is the energy needed to remove one particle from the bound state of a system of N particles. The HVZ theorem tells us that $E_N \leq E_{N-1}$, and if $E_N < E_{N-1}$ then H_N has a ground state (by the Min-max principle).

Proof of HVZ theorem. We will use Weyl's criterion theorem. For simplicity we consider the case when H_N acts on the full space $L^2(\mathbb{R}^{dN})$; the bosonic and fermionic cases follow small modifications.

Step 1. We prove that $[E_{N-1}, \infty) \subset \sigma_{\text{ess}}(H_N)$. In this step we do not need $W \geq 0$.
We take $\lambda \geqslant 0$ and prove that

$$E_{N-1} + \lambda \in \sigma_{\text{ess}}(H_N).$$

By Weyl's theorem, we need to find a Weyl sequence $\{\Psi_N^{(n)}\}_{n\geq 1} \subset L^2(\mathbb{R}^{dN})$ such that

$$\|\Psi_N^{(n)}\| = 1, \quad \Psi_N^{(n)} \rightharpoonup 0, \quad \|(H_N - E_{N-1} - \lambda)\Psi_N^{(n)}\| \to 0 \quad as \quad n \to \infty.$$

The choice of the Weyl sequence:

- Since $E_{N-1} = \inf \sigma(H_{N-1})$, we have $E_{N-1} \in \sigma(H_{N-1})$ (**the spectrum is closed**). Therefore, by Weyl's theorem, there exists a Weyl sequence $\{\Psi_{N-1}^{(n)}\}_{n\geq 1} \subset L^2(\mathbb{R}^{d(N-1)})$ such that

$$\|\Psi_{N-1}^{(n)}\| = 1, \quad \|(H_{N-1} - E_{N-1})\Psi_{N-1}^{(n)}\| \to 0 \quad as \quad n \to \infty.$$

- Since $\lambda \geq 0$, we have $\lambda \in \sigma_{\text{ess}}(-\Delta_{\mathbb{R}^d})$. Therefore, by Weyl's theorem, there exists a sequence $\{u^{(n)}\} \subset L^2(\mathbb{R}^d)$ such that

$$\|u^{(n)}\| = 1, \quad u^{(n)} \rightharpoonup 0, \quad \|(-\Delta_{\mathbb{R}^d} - \lambda)u^{(n)}\| \to 0 \quad as \quad n \to \infty.$$

- Then we can choose

$$\Psi_N^{(n)} = \Psi_{N-1}^{(n)} \otimes u^{(n)},$$

  namely

$$\Psi_N^{(n)}(x_1, ..., x_N) = \Psi_{N-1}^{(n)}(x_1, ..., x_{N-1})u^{(n)}(x_N).$$

  It remains to check that $\{\Psi_N^{(n)}\}_{n\geq 1}$ is a desired Weyl's sequence for H_N. It is actually correct. However, to make the proof easier, let us refine the choice of $\Psi_{N-1}^{(n)}$ and $u^{(n)}$ a bit: by a standard density argument we can choose such that

$$\operatorname{supp} \Psi_{N-1}^{(n)} \subset B_{\mathbb{R}^{dN}}(0, R_n), \quad \operatorname{supp} u^{(n)} \subset \{x \in \mathbb{R}^d : 2R_n \leq |x| \leq 3R_n\}$$

  for some sequence $R_n \geq 4R_{n-1}$ (you should check why?).

Now let us prove that $\Psi_N^{(n)} = \Psi_{N-1}^{(n)} \otimes u^{(n)}$ is a good choice. First,

$$\|\Psi_N^{(n)}\| = \|\Psi_{N-1}^{(n)}\|\|u^n\| = 1.$$

Moreover, since the functions $\{u^{(n)}\}$ have disjoint supports, the functions $\{\Psi_N^{(n)}\}_{n\geq 1}$ also have disjoint supports. In particular, $\{\Psi_N^{(n)}\}_{n\geq 1}$ is an orthonormal family, and hence

$$\Psi_N^{(n)} \rightharpoonup 0 \quad \text{weakly in } L^2(\mathbb{R}^{dN}).$$

Next, we decompose

$$H_N = H_{N-1} + (-\Delta_{x_N}) + V(x_N) + \sum_{i=1}^{N-1} W(x_i - x_N).$$

Therefore, by the triangle inequality

$$\begin{aligned}\|(H_N - E_{N-1} - \lambda)\Psi_N^{(n)}\| &\le \|(H_{N-1} - E_{N-1})\Psi_N^{(n)}\| + \|(-\Delta_{x_N} - \lambda)\Psi_N^{(n)}\| \\ &\quad + \|V(x_N)\Psi_N^{(n)}\| + \sum_{i=1}^{N-1} \|W(x_i - x_N)\Psi_N^{(n)}\|.\end{aligned}$$

We have

$$\begin{aligned}\|(H_{N-1} - E_{N-1})\Psi_N^{(n)}\| &= \|(H_{N-1} - E_{N-1})\Psi_{N-1}^{(n)}\|\|u^{(n)}\| \to 0, \\ \|(-\Delta_{x_N} - \lambda)\Psi_N^{(n)}\| &= \|\Psi_{N-1}^{(n)}\|\|(-\Delta - \lambda)u^{(n)}\| \to 0, \\ \|V(x_N)\Psi_N^{(n)}\| &= \|\Psi_{N-1}^{(n)}\|\|Vu^{(n)}\| = \|V(x)\mathbb{1}(|x| \ge 2R_n)u^{(n)}\| \to 0, \\ \|W(x_i - x_N)\Psi_N^{(n)}\| &= \|W(x_i - x_N)\mathbb{1}(|x_i - x_N| \ge R_n)\Psi_{N-1}^{(n)}u^{(n)}\| \to 0.\end{aligned}$$

For the last two convergences are obvious if we know that $V(x) \to 0, W(x) \to 0$ as $|x| \to \infty$. More generally, if $V, W \in L^p + L^q$, then we can use Hölder and Sobolev inequalities as in the proof of the self-adjointness, plus the fact that

$$\|V(x)\mathbb{1}(|x| \ge 2R_n)\|_{L^p+L^q} \to 0, \quad \|W(x)\mathbb{1}(|x| \ge R_n)\|_{L^p+L^q} \to 0.$$

Here $u^{(n)}$ is bounded in $H^2(\mathbb{R}^d)$.

This concludes the proof of $[E_{N-1}, \infty) \subset \sigma_{\text{ess}}(H_N)$.

Step 2. Now we prove that $\sigma_{\text{ess}}(H_N) \subset [E_{N-1}, \infty)$. In this step we need $W \ge 0$.

Take $\lambda + E_{N-1} \in \sigma_{\text{ess}}(H_N)$. We prove that $\lambda \ge 0$. By Weyl's theorem, there exists a Weyl sequence $\{\Psi_N^{(n)}\}_{n\ge1} \subset L^2(\mathbb{R}^{dN})$ such that

$$\|\Psi_N^{(n)}\| = 1, \quad \Psi_N^{(n)} \rightharpoonup 0, \quad \|(H_N - E_{N-1} - \lambda)\Psi_N^{(n)}\| \to 0 \quad as \quad n \to \infty.$$

From the above properties, we find that $\{\Psi_N^{(n)}\}$ is bounded in $H^2(\mathbb{R}^{dN})$, and hence the weak convergence in L^2 can be upgraded to $\Psi_N^{(n)} \rightharpoonup 0$ in $H^2(\mathbb{R}^{dN})$ (see the exercise below). By Sobolev compact embedding theorem, we find that up to a subsequence as $n \to \infty$, we can find $R_n \to \infty$ such that

$$\|\Psi_N^{(n)} \mathbb{1}_{B(0,NR_n)}\| \to 0.$$

Physically, the latter convergence shows that $\Psi_N^{(n)}$ is not localized, namely at least one of N particles must **escape to infinity**. To trace the behavior at infinity, we use the IMS localization technique.

- We choose two smooth functions $\chi, \eta : \mathbb{R}^d \to \mathbb{R}$ such that

$$\chi^2 + \eta^2 = \mathbb{1}_{\mathbb{R}^d}, \quad \operatorname{supp} \chi \subset \{|x| \le R_n\}, \quad \operatorname{supp} \eta \subset \{|x| \ge R_n/2\}, \quad |\nabla \chi| + |\nabla \eta| \le \frac{C}{R_n}.$$

- On $\mathbb{R}^{dN}$ we have the partition of unity

$$\begin{aligned}\mathbb{1}_{\mathbb{R}^{dN}} &= \eta^2(x_1) + \chi^2(x_1) = \eta^2(x_1) + \eta^2(x_2)\chi^2(x_1) + \chi^2(x_2)\chi^2(x_1) \\ &= \eta^2(x_1) + \eta^2(x_2)\chi^2(x_1) + \eta^2(x_3)\chi^2(x_2)\chi^2(x_1) + ... + \chi^2(x_N)...\chi^2(x_1) \\ &=: \sum_{j=1}^N \varphi_j^2 + \varphi_0^2.\end{aligned}$$

  Then we have $|\nabla \varphi_j| \le C_N/R_n$ for all $j \ge 0$ and

$$\operatorname{supp} \varphi_0 \subset B_{\mathbb{R}^{dN}}(0, NR_n), \quad \operatorname{supp} \varphi_j \subset \{|x_j| \ge R_n/2\} \quad \text{for all } j \ge 1.$$

Next we apply the IMS formula for $\varphi_0, ..., \varphi_N$:

$$H_N = \sum_{j=0}^N \varphi_j H_N \varphi_j - \sum_{j=0}^N |\nabla \varphi_j|^2 \ge \sum_{j=0}^N \varphi_j H_N \varphi_j - \frac{C_N}{R_n^2}.$$

Therefore, by the choice of $\Psi_N^{(n)}$:

$$E_{N-1} + \lambda = \lim_{n\to\infty} \langle \Psi_N^{(n)}, H_N \Psi_N^{(n)} \rangle \ge \liminf_{n\to\infty} \sum_{j=0}^N \langle \Psi_N^{(n)}, \varphi_j H_N \varphi_j \Psi_N^{(n)} \rangle.$$

To conclude, let us show that for any $j = 0, 1, 2, ..., N$, we have

$$\langle \Psi_N^{(n)}, \varphi_j H_N \varphi_j \Psi_N^{(n)} \rangle \ge E_{N-1} \|\varphi_j \Psi_N^{(n)}\|^2 + o(1)_{n\to\infty}.$$

For $j=0$, using $\varphi_0 H_N \varphi_0 \geq E_N \varphi_0^2$ and the fact $\|\Psi_N^{(n)} \mathbb{1}_{B(0,R_n)}\| \to 0$ we get

$$\langle \Psi_N^{(n)}, \varphi_0 H_N \varphi_0 \Psi_N^{(n)} \rangle \geq E_N \|\varphi_0 \Psi_N^{(n)}\|^2 \to 0 \quad as \quad n \to \infty.$$

Therefore, we can also write

$$\langle \Psi_N^{(n)}, \varphi_0 H_N \varphi_0 \Psi_N^{(n)} \rangle \geq E_{N-1} \|\varphi_0 \Psi_N^{(n)}\|^2 + o(1)_{n\to\infty}.$$

For $j=N$ we decompose

$$H_N = H_{N-1} + (-\Delta_{x_N}) + V(x_N) + \sum_{i=1}^{N} W(x_i - x_N) \geq E_{N-1} + V(x_N)$$

(**here we use** $W \geq 0$). Therefore,

$$\varphi_N H_N \varphi_N \geq E_{N-1} \varphi_N^2 - |V(x_N) \mathbb{1}(|x_N| \geq R_n/2)|.$$

Thus

$$\begin{aligned} \langle \Psi_N^{(n)}, \varphi_j H_N \varphi_j \Psi_N^{(n)} &\geq E_{N-1} \|\varphi_N \Psi_N^{(n)}\|^2 + \langle \Psi_N^{(n)}, |V(x_N) \mathbb{1}(|x_N| \geq R_n/2)| \Psi_N^{(n)} \rangle \\ &\geq E_{N-1} \|\varphi_N \Psi_N^{(n)}\|^2 + o(1)_{n\to\infty}. \end{aligned}$$

Of course the same bound holds for $j = 1, 2, ..., N-1$ as well. In summary, we have proved that

$$E_{N-1} + \lambda \geq \liminf_{n\to\infty} \sum_{j=0}^{N} \langle \Psi_N^{(n)}, \varphi_j H_N \varphi_j \Psi_N^{(n)} \rangle \geq \liminf_{n\to\infty} \sum_{j=0}^{N} E_{N-1} \|\varphi_j \Psi_N^{(n)}\|^2 = E_{N-1}.$$

Thus $\lambda \geq 0$. This ends the proof of $\sigma_{\rm ess}(H_N) \subset [E_{N-1}, \infty)$.

So far we have proved $\sigma_{\rm ess}(H_N) = [E_{N-1}, \infty)$ when H_N acts on the full space $L^2(\mathbb{R}^{dN})$. When H_N acts on the bosonic/fermionic space $L^2(\mathbb{R}^d)^{\otimes_{s/a} N}$ we can proceed exactly the same, except that in the direction $[E_{N-1}, \infty) \subset \sigma_{\rm ess}(H_N)$ we should choose the Weyl sequence as

$$\Psi_N^{(n)} = P_{\pm} \Psi_{N-1}^{(n)} \otimes u^{(n)} \in L^2(\mathbb{R}^d)^{\otimes_{s/a} N}.$$

q.e.d.

Exercise. *Let $\mathscr{H}_1$ and $\mathscr{H}_2$ be two Hilbert spaces such that $\mathscr{H}_2 \subset \mathscr{H}_1$ and*

$$\|u\|_{\mathscr{H}_2} \geq \|u\|_{\mathscr{H}_1}, \quad u \in \mathscr{H}_2.$$

Assume that the sequence $\{u_n\}_{n\geq 1}$ is bounded in $\mathscr{H}_2$ and $u_n \rightharpoonup 0$ in $\mathscr{H}_1$. Prove that $u_n \rightharpoonup 0$ in $\mathscr{H}_2$.

2.8 How many electrons that a nucleus can bind?

Now we take a closer look at the **Atomic Hamiltonian**

$$H_N^{\text{atom}} = \sum_{i=1}^{N} \Big(-\Delta_{x_i} - \frac{Z}{|x_i|} \Big) + \sum_{1 \leq i < j \leq N} \frac{1}{|x_i - x_j|}$$

which describes a system of N **quantum electrons** of charge -1 moving around a **classical nucleus** of charge $Z > 0$ fixed at the origin in $\mathbb{R}^3$. The particles interact via the **Coulomb potential**. Physically, the Hamiltonian H_N^{atom} is an operator on the fermionic space $L^2(\mathbb{R}^3)^{\otimes_a N}$ (**electrons are fermions**). Mathematically, we may also consider H_N^{atom} as an operator on $L^2(\mathbb{R}^{3N})$ or $L^2(\mathbb{R}^3)^{\otimes_s N}$. We will consider the nuclear charge $Z > 0$ as an arbitrary positive number, although it is an integer in practice.

In this section, we address the following question: for a given nuclear charge Z, is there a ground state for H_N? i.e. "**how many electron that a nucleus can bind?**". From experimental chemistry, it is observed that a nucleus of charge Z can bind up to $Z+1$ or $Z+2$, but higher negative ions do not exist. Proving this fact rigorously for the Hamiltonian H_N^{atom} is a long-standing problem in mathematical physics, call the **ionization conjecture**. In the following, we will represent two fundamental results, one for the existence (Zhilin's theorem) and one for the non-existence (Lieb's theorem).

Recall that from Kato's theorem, we know that H_N^{atom} is self-adjoint with domain $H^2(\mathbb{R}^{3N})$ or $H^2_{a/s}(\mathbb{R}^{3N})$, and that its ground state energy

$$E_N := \inf \sigma(H_N^{\text{atom}})$$

is finite. Moreover, from the HVZ theorem we know that

$$\sigma_{\rm ess}(H_N^{\rm atom}) = [E_{N-1}, \infty)$$

where E_{N-1} is the ground state energy of $H_{N-1}^{\rm atom}$ (with the same nuclear charge Z). Consequently, $H_N^{\rm atom}$ has a ground state if we have the **strict binding inequality** $E_N < E_{N-1}$. In principle, when $E_N = E_{N-1}$, $H_N^{\rm atom}$ may still have a ground state (although the ground state is very unstable as one particle can escape to infinity without losing any energy).

Theorem (Zhilin's Existence Theorem)**.** *Consider $H_N^{\rm atom}$ as an operator on $L^2(\mathbb{R}^{3N})$ or $L^2(\mathbb{R}^3)^{\otimes_{a/s} N}$. For any $1 \le N < Z+1$, we have the* **strict binding inequality** *$E_N < E_{N-1}$. Consequently, the Hamiltonian $H_N^{\rm atom}$ has a ground state.*

Proof. We will prove $E_N < E_{N-1}$ by induction. This holds for $N = 1$ as $E_1 = -\frac{1}{4} < 0$ (the hydrogen atom). Assume that we have proved $E_{N-1} < E_{N-2}$ for some $N < Z$. Now we show that $E_N < E_{N-1}$. By the variational principle, we need to find a wave function Ψ_N such that

$$\langle \Psi_N, H_N^{\rm atom} \Psi_N \rangle < E_{N-1}.$$

Let us consider the case when $H_N^{\rm atom}$ acts on $L^2(\mathbb{R}^{3N})$; the bosonic and fermionic cases follow simple modifications.

- From the induction hypothesis $E_{N-1} < E_{N-2}$ and the HVZ theorem, we know that $H_{N-1}^{\rm atom}$ has a ground state $\Psi_{N-1} \in L^2(\mathbb{R}^{3(N-1)})$.
- Take a smooth function $\varphi : \mathbb{R}^3 \to \mathbb{R}$ with $\operatorname{supp} \varphi \subset \{x \in \mathbb{R}^3 : 1 < |x| < 2\}$ and $\|\varphi\|_{L^2(\mathbb{R}^3)} = 1$. For any $R > 0$ we choose

  $$\varphi_R(x) = \frac{1}{R^{3/2}} \varphi\Big(\frac{x}{R}\Big).$$

  Then

  $$\operatorname{supp} \varphi_R \subset \{x \in \mathbb{R}^3 : R \le |x| \le 2R\}, \quad \|\varphi_R\|_{L^2} = 1.$$

- We choose the trial state

  $$\Psi_N = \Psi_{N-1} \otimes \varphi_R \in L^2(\mathbb{R}^{3N}).$$

Then

$$\|\Psi_N\|_{L^2(\mathbb{R}^{3N})} = \|\Psi_{N-1}\|_{L^2(\mathbb{R}^{3(N-1)})}\|\varphi_R\|_{L^2(\mathbb{R}^3)} = 1.$$

It remains to show that $\langle \Psi_N, H_N^{\text{atom}} \Psi_N \rangle < E_{N-1}$.

Similarly to the proof of the HVZ theorem, we decompose

$$H_N^{\text{atom}} = H_{N-1}^{\text{atom}} + \Big(-\Delta_{x_N} - \frac{Z}{|x_N|} + \sum_{i=1}^{N-1} \frac{1}{|x_i - x_N|} \Big).$$

Therefore,

$$\langle \Psi_N, H_N^{\text{atom}} \Psi_N \rangle = E_{N-1} + \|\nabla \varphi_R\|^2_{L^2(\mathbb{R}^3)} - \int_{\mathbb{R}^3} \frac{Z|\varphi_R(x)|^2}{|x|} \mathrm{d}x$$
$$+ \sum_{i=1}^{N-1} \int_{\mathbb{R}^{3N}} \frac{1}{|x_i - x_N|} |\Psi_{N-1}(x_1, ..., x_{N-1})|^2 |\varphi_R(x_N)|^2 \mathrm{d}x_1 ... \mathrm{d}x_N.$$

By the choice of φ_R, we have

$$\|\nabla \varphi_R\|^2_{L^2(\mathbb{R}^3)} = \frac{1}{R^2} \|\nabla \varphi\|^2_{L^2(\mathbb{R}^3)}$$

and

$$-\int_{\mathbb{R}^3} \frac{Z|\varphi_R(x)|^2}{|x|} \mathrm{d}x = -\frac{Z}{R} \int_{\mathbb{R}^3} \frac{Z|\varphi(x)|^2}{|x|} \mathrm{d}x.$$

Moreover, by **Newton's theorem**

$$\int_{\mathbb{R}^3} \frac{|\varphi_R(x)|^2}{|y-x|} \mathrm{d}x = \int_{\mathbb{R}^3} \frac{|\varphi_R(x)|^2}{\max(|y|, |x|)} \mathrm{d}x \leq \int_{\mathbb{R}^3} \frac{|\varphi_R(x)|^2}{|x|} \mathrm{d}x = \int_{\mathbb{R}^3} \frac{|\varphi(x)|^2}{R|x|} \mathrm{d}x.$$

Consequently,

$$\sum_{i=1}^{N-1} \int_{\mathbb{R}^{3N}} \frac{1}{|x_i - x_N|} |\Psi_{N-1}(x_1, ..., x_{N-1})|^2 |\varphi_R(x_N)|^2 \mathrm{d}x_1 ... \mathrm{d}x_N$$
$$= \sum_{i=1}^{N-1} \int_{\mathbb{R}^{3N-1}} |\Psi_{N-1}(x_1, ..., x_{N-1})|^2 \Big(\int_{\mathbb{R}^3} \frac{|\varphi_R(x_N)|^2}{|x_i - x_N|} \mathrm{d}x_N \Big) \mathrm{d}x_1 ... \mathrm{d}x_{N-1}$$
$$\leq \sum_{i=1}^{N-1} \int_{\mathbb{R}^{3N-1}} |\Psi_{N-1}(x_1, ..., x_{N-1})|^2 \Big(\int_{\mathbb{R}^3} \frac{|\varphi(x)|^2}{R|x|} \mathrm{d}x \Big) \mathrm{d}x_1 ... \mathrm{d}x_{N-1}$$
$$= \frac{N-1}{R} \int_{\mathbb{R}^3} \frac{|\varphi(x)|^2}{|x|} \mathrm{d}x.$$

In summary, we obtain

$$\langle \Psi_N, H_N^{\text{atom}} \Psi_N \rangle \le E_{N-1} + \frac{1}{R^2} \|\nabla \varphi\|^2_{L^2(\mathbb{R}^3)} + \frac{N-1-Z}{R} \int_{\mathbb{R}^3} \frac{|\varphi(x)|^2}{|x|} \mathrm{d}x.$$

Under the condition $N < Z+1$, i.e. $N-1-Z<0$, for $R>0$ sufficiently large we have

$$\frac{1}{R^2} \|\varphi\|^2_{L^2(\mathbb{R}^3)} + \frac{N-1-Z}{R} \int_{\mathbb{R}^3} \frac{|\varphi(x)|^2}{|x|} \mathrm{d}x < 0,$$

which implies that

$$E_N \le \langle \Psi_N, H_N^{\text{atom}} \Psi_N \rangle < E_{N-1}.$$

This concludes the proof when H_N^{atom} acts on $L^2(\mathbb{R}^{3N})$. When H_N^{atom} acts on $L^2(\mathbb{R}^3)^{\otimes_{a/s} N}$ we choose

$$\Psi_N = P_{\pm} \Psi_{N-1} \otimes \varphi_R \in L^2(\mathbb{R}^3)^{\otimes_{a/s} N}$$

and proceed similarly. *q.e.d.*

In the above proof we have used

Theorem (Newton's theorem)**.** *Let μ be a positive measure on $\mathbb{R}^3$ such that it is* **radially symmetric***, namely $\mathrm{d}\mu(\mathcal{R}x) = \mathrm{d}\mu(x)$ for any rotation $\mathcal{R} \in SO(3)$. Then we have*

$$\int_{\mathbb{R}^3} \frac{\mathrm{d}\mu(x)}{|y-x|} = \int_{\mathbb{R}^3} \frac{\mathrm{d}\mu(x)}{\max(|y|,|x|)}, \quad \forall y \in \mathbb{R}^3.$$

Newton's theorem follows from the fact that the Coulomb potential is the Green function of Laplacian, namely

$$-\Delta(4\pi|x|)^{-1} = \delta_0 \quad (\text{the } \textbf{Dirac-delta distribution}).$$

In fact, here we only need $\Delta(|x|^{-1}) = 0$ for all $x \neq 0$ (which can be checked easily), namely $|x|^{-1}$ is a **harmonic function** on $\mathbb{R}^3 \backslash \{0\}$. The **Mean-value theorem** states that the average value of a harmonic function over a ball or sphere is equal to its value at the center.

Exercise. *Consider H_N^{atom} as an operator on $L^2(\mathbb{R}^{3N})$ or $L^2(\mathbb{R}^3)^{\otimes_{a/s} N}$. Prove that if $1 \le N < Z+1$, then H_N^{atom} has* **infinitely many eigenvalues** *below the essential spectrum.*

Theorem (Lieb's Nonexistence Theorem)**.** *If $N \geq 2Z+1$, then the Hamiltonian $H_N^{\rm atom}$* **does not** *have a ground state on $L^2(\mathbb{R}^{3N})$ or $L^2(\mathbb{R}^3)^{\otimes_{a/s} N}$.*

Proof. Assume that H_N has a ground state Ψ_N. Then it satisfies the Schrödinger equation

$$H_N \Psi_N = E_N \Psi_N.$$

Multiplying the Schrödinger equaiton with $|x_N|\overline{\Psi_N}$ and integrating we get

$$\begin{aligned} 0 &= \langle |x_N|\Psi_N, (H_N - E_N)\Psi_N\rangle = \\ &= \Big\langle |x_N|\Psi_N, \Big(H_{N-1}^{\rm atom} - E_N - \Delta_{x_N} - \frac{Z}{|x_N|} + \sum_{i=1}^{N-1} \frac{1}{|x_i - x_N|}\Big)\Psi_N \Big\rangle. \end{aligned}$$

We have

- $\big\langle |x_N|\Psi_N, (H_{N-1}^{\rm atom} - E_N)\Psi_N\big\rangle \geq 0$. This follows from $H_{N-1}^{\rm atom} \geq E_{N-1} \geq E_N$ on the $(N-1)$-particle space, by the HVZ theorem.

- $\langle |x_N|\Psi_N, -\Delta_{x_N}\Psi_N\rangle = \frac{1}{2}\Big\langle \Psi_N, \Big(|x_N|(-\Delta_{x_N}) + (-\Delta_{x_N})|x_N|\Big)\Psi_N\Big\rangle \geqslant 0$ (**the left side is real, why?**). This follows from the IMS formula and Hardy's inequality

$$\begin{aligned} \frac{(-\Delta)|x| + |x|(-\Delta)}{2} &= |x|^{1/2}(-\Delta)|x|^{1/2} - |\nabla(|x|^{1/2})|^2 \\ &= |x|^{1/2}(-\Delta)|x|^{1/2} - \Big|\frac{1}{2|x|^{1/2}}\Big|^2 \\ &= |x|^{1/2}\Big(-\Delta - \frac{1}{4|x|^2}\Big)|x|^{1/2} \geq 0 \quad \text{ on } L^2(\mathbb{R}^3). \end{aligned}$$

Thus

$$0 \geqslant -Z + \sum_{i=1}^{N-1} \int_{\mathbb{R}^{3N}} \frac{|x_N|}{|x_i - x_N|}|\Psi_N|^2 \iff Z \geqslant \sum_{i=1}^{N-1} \int_{\mathbb{R}^{3N}} \frac{|x_N|}{|x_i - x_N|}|\Psi_N|^2.$$

Similarly we get for all $j \in \{1, \ldots, N\}$

$$Z \geqslant \sum_{i: i \neq j} \int \frac{|x_j|}{|x_i - x_j|}|\Psi_N|^2$$

Averaging over $j \in \{1, \dots, N\}$ we get

$$Z \geqslant \frac{1}{N} \sum_{\substack{1 \le i,j \le N \\ i \neq j}}^{N} \int \frac{|x_j|}{|x_i - x_j|} |\Psi_N|^2 = \frac{1}{2N} \sum_{\substack{1 \le i,j \le N \\ i \neq j}}^{N} \int \underbrace{\frac{|x_i| + |x_j|}{|x_i - x_j|}}_{\geqslant 1} |\Psi_N|^2 > \frac{1}{2N} \sum_{\substack{1 \le i,j \le N \\ i \neq j}}^{N} 1 = \frac{N-1}{2}.$$

Thus $Z > \frac{N-1}{2}$, i.e. $N < 2Z + 1$. Here we have the strict inequality at the end because

$$\sum_{1 \le i,j \le N i \neq j} \frac{|x_i| + |x_j|}{|x_i - x_j|} > 1$$

for a.e. $(x_1, ..., x_N) \in \mathbb{R}^{3N}$. *q.e.d.*

Remarks:

- For $Z = 1$ (hydrogen atom), Lieb's theorem implies that the negative ion H^{--} does not exist. This is sharp because it is known (mathematically) that H^- exists.

- For larger Z, the factor 2 in Lieb's bound is not sharp. For **fermionic ground states**, the above proof can be modified by multiplying the Schrödinger equation with $|x_N|^2 \overline{\Psi_N}$ instead of $|x_N| \overline{\Psi_N}$, leading to the non-existence when (my paper)

$$N \geq 1.22Z + 3Z^{1/3}.$$

  When $Z \to \infty$, the non-existence of fermionic ground states is known when

$$N \geq (1 + \varepsilon)Z$$

  for any $\varepsilon > 0$. This so-called **asymptotic neutrality** was first proved by Lieb, Sigal, Simon, and Thirring (PRL 1984) and improved later in (CMP 1990a, CMP 1990b). The non-existence of fermionic ground states when

$$N \geq Z + C$$

  for a universal constant C (possibly $C = 2$) remains an **open problem**.

- When H_N^{atom} acts on the full space $L^2(\mathbb{R}^{3N})$ or the bosonic space $L^2(\mathbb{R}^3)^{\otimes_s N}$, a ground state exists up to $N \sim 1.21Z$. This was proved by Benguria and Lieb (PRL 1983). This is an evidence that the particle statistics changes dramatically the spectral properties of the quantum system.

Chapter 3

Hartree theory

Definition. *Let* $V : \mathbb{R}^d \to \mathbb{R}$ *and* $w : \mathbb{R}^d \to R$ *even. We define the* **Hartree functional**

$$\mathcal{E}_{\mathrm{H}}(u) := \int_{\mathbb{R}^d} \Big(|\nabla u(x)|^2 + V(x)|u(x)|^2\Big)\mathrm{d}x + \frac{1}{2}\iint_{\mathbb{R}^d\times\mathbb{R}^d} |u(x)|^2|u(y)|^2 w(x-y)\mathrm{d}x\mathrm{d}y$$

and the **Hartree energy**

$$e_{\mathrm{H}} := \inf\{\mathcal{E}_{\mathrm{H}}(u) : u \in H^1(\mathbb{R}^d), \|u\|_{L^2(\mathbb{R}^d)} = 1\}.$$

If a **Hartree minimizer** u_0 *exists, then it satisfies the* **Hartree equation**

$$\Big(-\Delta + V(x) + (w * |u_0|^2)(x) - \mu\Big)u_0(x) = 0, \quad x \in \mathbb{R}^d$$

for a constant $\mu \in \mathbb{R}$ *(called the* **Lagrange multiplier** *or* **chemical potential***).*

The Hartree equation is also often called the **Gross-Pitaaevskii equation** or **nonlinear Schrödinger equation**, in particular when $w = a\delta_0$ (Dirac-delta distribution). In this case, the functional becomes

$$\mathcal{E}_{\mathrm{H}}(u) := \int_{\mathbb{R}^d} \Big(|\nabla u(x)|^2 + V(x)|u(x)|^2\Big) + \frac{a}{2}\iint_{\mathbb{R}^d} |u(x)|^4 dx$$

and its minimizer satisfies

$$\Big(-\Delta + V(x) + a|u_0(x)|^2 - \mu\Big)u_0(x) = 0, \quad x \in \mathbb{R}^d.$$

The Hartree/GP/NLS equation is an important topic in many areas of mathematics, e.g. nonlinear analysis, calculus of variations, and partial differential equations. In this chapter we study basic properties of Hartree theory and in the next chapter we discuss its connection to quantum Bose gases.

Connection to many-body quantum mechanics. Consider a system of N **identical bosons** in $\mathbb{R}^d$, described by the Hamilttonian

$$H_N = \sum_{i=1}^{N} (-\Delta_{x_i} + V(x_i)) + \sum_{1\le i<j\le N} W(x_i - x_j)$$

acting on $L^2(\mathbb{R}^d)^{\otimes_s N}$. As usual, $V, W : \mathbb{R}^d \to \mathbb{R}$ and W is even.

Since the underlying Hilbert space is too large, it is often useful to restrict the consideration to the Hartree states

$$\Psi = u^{\otimes N}, \quad \|u\|_{L^2(\mathbb{R}^d)} = 1.$$

The corresponding energy expectation (per particle) is exactly given by the Hartree functional

$$\frac{1}{N}\langle u^{\otimes N}, H_N u^{\otimes N}\rangle = \int_{\mathbb{R}^d} \Big(|\nabla u(x)|^2 + V(x)|u(x)|^2\Big) + \frac{1}{2}\iint |u(x)|^2 |u(y)|^2 w(x-y)dxdy =: \mathcal{E}_{\rm H}(u)$$

with $w = (N-1)W$. By the variational principle, the Hartree energy is always an upper bound to the ground state energy (per particle) of the full N-body problem, namely

$$E_N := \inf_{\|\Psi\|_{L^2(\mathbb{R}^d)^{\otimes_s N}}=1} \langle \Psi, H_N \Psi\rangle \le N e_{\rm H}.$$

The matching lower bound is nontrivial. We will prove that, under appropriate conditions on the potentials,

$$E_N = N e_{\rm H} + o(N).$$

Moreover, we will prove that Hartree minimizers will give the leading order information to the ground states of the N-body problem, leading to a rigorous justification of the **Bose-Einstein condensation** for some weakly interacting bosonic systems.

3.1 Existence of minimizers: trapping potentials

Theorem (Existence of Hartree minimizers: trapping case)**.** *Consider the Hartree functional*

$$\mathcal{E}_{\mathrm{H}}(u) := \int_{\mathbb{R}^d} \left(|\nabla u(x)|^2 + V(x)|u(x)|^2\right)\mathrm{d}x + \frac{1}{2}\iint_{\mathbb{R}^d\times\mathbb{R}^d} |u(x)|^2|u(y)|^2 w(x-y)\mathrm{d}x\mathrm{d}y$$

with

- $w \in L^p(\mathbb{R}^d) + L^\infty(\mathbb{R}^d)$ *with* $p > \max(d/2, 1)$,
- $V \in L^p_{\mathrm{loc}}(\mathbb{R}^d)$ *and* $V(x) \to +\infty$ *as* $|x| \to \infty$.

Then the minimization problem

$$e_{\mathrm{H}} := \inf\left\{\mathcal{E}_{\mathrm{H}}(u) : u \in H^1(\mathbb{R}^d), \|u\|_{L^2(\mathbb{R}^d)} = 1\right\}$$

has a minimizer (in particular e_{H} *is finite).*

Proof. We use the direct method of **Calculus of variations**.

Step 1 (Boundedness from below). Let $u \in H^1(\mathbb{R}^d)$ with $\|u\|_{L^2(\mathbb{R}^d)} = 1$. For any $\varepsilon > 0$ we can write

$$w = w_1 + w_2, \quad \|w_1\|_{L^p(\mathbb{R}^d)} \le \varepsilon, \quad \|w_2\|_{L^\infty(\mathbb{R}^d)} \le C_\varepsilon.$$

Then

$$\iint_{\mathbb{R}^d\times\mathbb{R}^d} |u(x)|^2|u(y)|^2|w_2(x-y)|\mathrm{d}x\mathrm{d}y \le \|w_2\|_{L^\infty}\iint |u(x)|^2|u(y)|^2\mathrm{d}x\mathrm{d}y \le C_\varepsilon.$$

Moreover, by Hölder and Young inequalities

$$\begin{aligned}\iint_{\mathbb{R}^d\times\mathbb{R}^d} |u(x)|^2|u(y)|^2|w_1(x-y)|\mathrm{d}x\mathrm{d}y &= \int |u(x)|^2(|w_1| * |u|^2)(x)\mathrm{d}x \\ &\le \||u|^2\|_{L^q}\||w_1| * |u|^2\|_{L^p} \\ &\le \|u\|^2_{L^{2q}}\|w_1\|_{L^p}\|u\|^2_{L^2}\end{aligned}$$

with

$$\frac{1}{p} + \frac{1}{q} = 1.$$

The condition $p > \max(d/2, 1)$ implies that $2q < 2^*$ where

$$2^* = \infty \text{ for } d \leq 2, \quad 2^* = \frac{2d}{d-2} \text{ for } d \geq 3.$$

By Sobolev inequality

$$\|u\|_{L^{2q}}^2 \leq C\|u\|_{H^1}^2 = C(\|\nabla u\|_{L^2}^2 + 1).$$

Thus

$$\iint_{\mathbb{R}^d \times \mathbb{R}^d} |u(x)|^2 |u(y)|^2 |w_1(x-y)| \mathrm{d}x\mathrm{d}y \leq \varepsilon C(\|\nabla u\|_{L^2}^2 + 1).$$

The total interaction energy is bounded by

$$\iint_{\mathbb{R}^d \times \mathbb{R}^d} |u(x)|^2 |u(y)|^2 |w(x-y)| \mathrm{d}x\mathrm{d}y \leq \varepsilon C\|\nabla u\|_{L^2}^2 + C_\varepsilon.$$

Similarly, for the external potential we write

$$V = V_1 + V_2, \quad \|V_1\|_{L^p(\mathbb{R}^d)} \leq \varepsilon, \quad V_2 \geq -C_\varepsilon, \quad \lim_{|x| \to \infty} V_2(x) = +\infty.$$

Using Hölder and Sobolev inequalities we get

$$\int_{\mathbb{R}^d} |V_1(x)||u(x)|^2 \mathrm{d}x \leq \varepsilon C(\|\nabla u\|_{L^2}^2 + 1).$$

By choosing ε small enough, we find that

$$\iint_{\mathbb{R}^d \times \mathbb{R}^d} |u(x)|^2 |u(y)|^2 |w(x-y)| \mathrm{d}x\mathrm{d}y + \int_{\mathbb{R}^d} |V_1(x)||u(x)|^2 \mathrm{d}x \leq \frac{1}{2}\|\nabla u\|_{L^2}^2 + C$$

for a constant C independent of u. Consequently, we get the lower bound

$$\mathcal{E}_{\mathrm{H}}(u) \geq \int_{\mathbb{R}^d} \left[\frac{1}{2}|\nabla u|^2 + V_2|u|^2\right] - C.$$

Since V_2 is bounded from below, we know that $\mathcal{E}_{\mathrm{H}}(u)$ is bounded from below uniformly in u. Thus e_{H} is finite.

Step 2 (Minimizing sequence). Since e_{H} is finite, there exists a minimizing sequence $\{u_n\}_{n\geq 1} \subset H^1(\mathbb{R}^d)$ for e_{H}, namely

$$\|u_n\|_{L^2(\mathbb{R}^d)} = 1, \quad \mathcal{E}_{\mathrm{H}}(u_n) \to e_{\mathrm{H}} \quad \text{as} \quad n \to \infty.$$

From the above lower bound, we find that

$$\int_{\mathbb{R}^d} \left[|\nabla u_n|^2 + 2V_2|u_n|^2 \right]$$

is bounded. Thus $\{u_n\}$ is bounded in the quadratic form domain of $Q(-\Delta+2V_2) = Q(-\Delta+V_2)$. By the Banach-Alaoglu theorem, up to a subsequence, we can assume that $u_n \rightharpoonup u_0$ weakly in $Q(-\Delta+V_2)$. We will show that u_0 is a minimizer for e_{H}.

Step 3 (Conservation of mass). The condition $V_2(x) \to +\infty$ as $|x| \to \infty$ implies that the operator $-\Delta + V_2$ has compact resolvent. Consequently, we have the compact embedding $Q(-\Delta+V_2) \subset L^2(\mathbb{R}^d)$ (exercise). Thus the weak convergence $u_n \rightharpoonup u_0$ in $Q(-\Delta+V_2)$ implies the strong convergence $u_n \to u_0$ in $L^2(\mathbb{R}^d)$. Therefore,

$$\|u_0\|_{L^2(\mathbb{R}^d)} = \lim_{n\to\infty} \|u_n\|_{L^2(\mathbb{R}^d)} = 1.$$

Step 4 (Semi-continuity). It remains to show that

$$\liminf_{n\to\infty} \mathcal{E}_{\mathrm{H}}(u_n) \geq \mathcal{E}_{\mathrm{H}}(u_0).$$

Since u_n is bounded in $Q(-\Delta+V_2) \subset H^1(\mathbb{R}^d)$ and $u_n \to u_0$ strongly in $L^2(\mathbb{R}^d)$, by interpolation (Sobolev's and Hölder inequalities) we find that $u_n \to u_0$ strongly in $L^q(\mathbb{R}^d)$ for all $2 \leq q < 2^*$ ($2^* = \infty$ if $d \leq 2$ and $2^* = 2d/(d-2)$ if $d \geq 3$). Consequently,

$$\lim_{n\to\infty} \iint |u_n(x)|^2|u_n(y)|^2 w(x-y)\mathrm{d}x\mathrm{d}y = \iint |u_0(x)|^2|u_0(y)|^2 w(x-y)\mathrm{d}x\mathrm{d}y.$$

(see an exercise below). Similarly, for the external potential $V = V_1 + V_2$, using $V_1 \in L^p(\mathbb{R}^d)$ we have

$$\lim_{n\to\infty} \int V_1(x)|u_n(x)|^2\mathrm{d}x = \int V_1(x)|u_0(x)|^2\mathrm{d}x$$

(see an exercise below). Finally, since $u_n \rightharpoonup u_0$ weakly in the quadratic form domain $Q(-\Delta+V_2)$, by Fatou's lemma for norms (see an exercise below) we have

$$\liminf_{n\to\infty} \int (|\nabla u_n|^2 + V_2|u_n|^2) \geq \int (|\nabla u_0|^2 + V_2|u_0|^2).$$

In summary,

$$e_{\mathrm{H}} = \liminf_{n\to\infty} \mathcal{E}_{\mathrm{H}}(u_n) \geq \mathcal{E}_{\mathrm{H}}(u_0).$$

This implies that u_0 is a minimizer for $e_{\rm H}$. *q.e.d.*

Exercise. *Let A be a positive self-adjoint operator on a Hilbert space $\mathscr{H}$ with compact resolvent. Prove that we have the compact embedding $Q(A) \subset \mathscr{H}$.*
Hint: By Spectral Theorem you can write $A = \sum_{n\ge 1} \lambda_n |u_n\rangle\langle u_n|$ with $\lambda_n \to \infty$. The identity $\mathbb{1} : Q(A) \to \mathscr{H}$ is a compact operator because it is the strong limit of finite-rank operators $B_n = \sum_{m=1}^n |u_m\rangle\langle u_m|$.

Exercise. *Let $V \in L^p(\mathbb{R}^d)$ with $p > \max(d/2, 1)$. Prove that if $u_n \rightharpoonup u_0$ weakly in $H^1(\mathbb{R}^d)$, then*

$$\lim_{n\to\infty} \int V(x)|u_n(x)|^2 {\rm d}x = \int V(x)|u_0(x)|^2 {\rm d}x.$$

Exercise. *Let $w \in L^p(\mathbb{R}^d)$ with $p > \max(d/2, 1)$. Let $\{u_n\}_{n\ge1}$, $\{v_n\}_{\ge1}$ be bounded sequences in $H^1(\mathbb{R}^d)$ such that $u_n \to u_0$ strongly in $L^2(\mathbb{R}^d)$ and $v_n \rightharpoonup v_0$ weakly in $L^2(\mathbb{R}^d)$. Prove that*

$$\lim_{n\to\infty} \iint_{\mathbb{R}^d\times\mathbb{R}^d} |u_n(x)|^2|v_n(y)|^2 w(x-y){\rm d}x{\rm d}y = \iint_{\mathbb{R}^d\times\mathbb{R}^d} |u_0(x)|^2|v_0(y)|^2 w(x-y){\rm d}x{\rm d}y.$$

Exercise. *(Fatou's lemma for norms) Assume that $v_n \rightharpoonup v$ weakly in a Hilbert space.*
1. Prove that

$$\liminf_{n\to\infty} \|v_n\| \ge \|v\|.$$

2. Prove that $\|v_n\| \to \|v\|$ if and only if $v_n \to v$ strongly.

3.2 Existence of minimizers: vanishing potentials

Now we turn to the case when the external potential V vanishes at infinity. This case is significantly more difficult since some mass may escape to infinity, leading to a possible lack of compactness. In fact, the existence of Hartree minimizers is not always guaranteed! We have to investigate all possibilities of losing mass at infinity. This is nicely done by the **concentration-compactness method** which has been developed since the 1980s by several people, including Lieb (Invent 1983) and Lions (AIHPC 1984a, AIHPC 1984b).

Theorem (Existence of Hartree minimizers: vanishing case)**.** *Consider the Hartree functional*

$$\mathcal{E}_{\rm H}^V(u) := \int_{\mathbb{R}^d} \Big(|\nabla u(x)|^2 + V(x)|u(x)|^2\Big)\mathrm{d}x + \frac{1}{2}\iint_{\mathbb{R}^d\times\mathbb{R}^d} |u(x)|^2|u(y)|^2 w(x-y)\mathrm{d}x\mathrm{d}y$$

with $w, V \in L^p(\mathbb{R}^d) + L^p(\mathbb{R}^d)$, $\max(d/2,1) < p,q < \infty$*. For any* $\lambda \in [0,1]$ *define*

$$e_{\rm H}^V(\lambda) := \inf\Big\{\mathcal{E}_{\rm H}^V(u) : u \in H^1(\mathbb{R}^d), \|u\|^2_{L^2(\mathbb{R}^d)} = \lambda\Big\}.$$

We denote by $e_{\rm H}^0(\lambda)$ *the corresponding energy with* $V = 0$ *("energy at infinity"). Then we always have the* **binding inequality**

$$e_{\rm H}^V(1) \le e_{\rm H}^V(\lambda) + e_{\rm H}^0(1-\lambda), \quad \forall \lambda \in [0,1]$$

Moreover, if we have the **strict binding inequality**

$$e_{\rm H}^V(1) < e_{\rm H}^V(\lambda) + e_{\rm H}^0(1-\lambda), \quad \forall \lambda \in [0,1),$$

then the variational problem $e_{\rm H}^V(1)$ *has a minimizer. In fact, for the existence of minimizers for* $e_{\rm H}^V(1)$*, we only need the strict binding inequality when* $e_{\rm H}^V(\lambda)$ *has a minimizer.*

Remarks:

- From the physical point of view, the binding inequality

$$e_{\rm H}^V(1) \le e_{\rm H}^V(\lambda) + e_{\rm H}^0(1-\lambda), \quad \forall \lambda \in [0,1]$$

  is rather obvious since the ground energy cannot be increased when we split the system into two parts: one with mass λ staying bounded, and one with mass $(1-\lambda)$ at infinity.

- The strict binding inequality

$$e_{\rm H}^V(1) < e_{\rm H}^V(\lambda) + e_{\rm H}^0(1-\lambda), \quad \forall \lambda \in [0,1)$$

  tells us that there is no possibility to put any positive mass at infinity (note that in the strict binding inequality we only requires $\lambda < 1$). It is a nontrivial condition and depends heavily on the potentials V, w.

- For repulsive interactions ($w \geq 0$), the energy at infinity is simply zero (see an exercise below). In this case, the binding inequality becomes

$$e_{\mathrm{H}}^{V}(1) \leq e_{\mathrm{H}}^{V}(\lambda), \quad \forall \lambda \in [0,1]$$

which is similar to the monotonicity $E_N \leq E_{N-1}$ in the HVZ theorem (both always hold true). The strict binding inequality

$$e_{\mathrm{H}}^{V}(1) < e_{\mathrm{H}}^{V}(\lambda), \quad \forall \lambda \in [0,1)$$

is thus similar to the binding condition $E_N < E_{N-1}$ in the N-body quantum problem.

Proof. **Step 1 (Boundedness from below).** By the same analysis of the trapping case, we have

$$\int_{\mathbb{R}^d} |V(x)||u(x)|^2 \mathrm{d}x + \frac{1}{2} \iint_{\mathbb{R}^d \times \mathbb{R}^d} |u(x)|^2 |u(y)|^2 |w(x-y)| \mathrm{d}x\mathrm{d}y \leq \frac{1}{2}\|\nabla u\|_{L^2}^2 + C$$

for all $u \in H^1(\mathbb{R}^d)$ with $\|u\|_{L^2} \leq 1$. Therefore,

$$\mathcal{E}_{\mathrm{H}}^{V}(u) \geq \frac{1}{2}\|\nabla u\|_{L^2}^2 - C.$$

This implies that $e_{\mathrm{H}}^{V}(\lambda)$ is finite for every $\lambda \in [0,1]$.

Step 2 (Binding inequality). Let $\lambda \in [0,1)$. By a standard density argument, we can find a sequence $\{a_n\}_{n \geq 1} \subset H^1(\mathbb{R}^d)$ such that

$$\mathrm{supp}(a_n) \subset \{|x| < n\}, \quad \int_{\mathbb{R}^d} |a_n|^2 = \lambda, \quad \mathcal{E}_{\mathrm{H}}^{V}(a_n) \leq e_{\mathrm{H}}^{V}(\lambda) + o(1)_{n \to \infty}.$$

(Explanation for the density argument: By the definition of $e_{\mathrm{H}}^{V}(\lambda)$, for any $\eta > 0$ small we can find a function $f_\eta \in H^1(\mathbb{R}^d)$ such that $\|f_\eta\|_{L^2}^2 = \lambda$ and $\mathcal{E}_{\mathrm{H}}^{V}(f_n) \leq e_{\mathrm{H}}^{V}(\lambda) + \eta$. Then since $C_c^1(\mathbb{R}^3)$ is dense in $H^1(\mathbb{R}^d)$ and the mapping $f \mapsto \mathcal{E}_{\mathrm{H}}(f)$ is continuous from $H^1(\mathbb{R}^d)$ to $\mathbb{R}$, we can replace f_η by $\widetilde{f_\eta} \in C_c^1(\mathbb{R}^3)$ with $\|\widetilde{f_\eta}\|_{L^2}^2 = \lambda$ and $\mathcal{E}_{\mathrm{H}}^{V}(\widetilde{f_\eta}) \leq e_{\mathrm{H}}^{V}(\lambda) + 2\eta$. By re-labeling $\eta \to 0$ by $n \to \infty$, we get the sequence $\{a_n\}$.)

Similarly, we can find a sequence $\{b_n\}_{n \geq 1} \subset H^1(\mathbb{R}^d)$ such that

$$\mathrm{supp}(b_n) \subset \{|x| > 2n\}, \quad \int_{\mathbb{R}^d} |b_n|^2 = 1 - \lambda, \quad \mathcal{E}_{\mathrm{H}}^{0}(b_n) \leq e_{\mathrm{H}}^{0}(1-\lambda) + o(1)_{n \to \infty}.$$

(Explanation for the choice of b_n: by the density argument, we can take b_n with compact support. Then since the functional $\mathcal{E}_{\rm H}^0(f)$ is translation-invariant (i.e. $\mathcal{E}_{\rm H}^0(f) = \mathcal{E}_{\rm H}^0(f(.-y))$ for any $y \in \mathbb{R}^d$) we can put the support of b_n inside $\{|x| > 2n\}$.)

Now we define the trial state

$$\varphi_n = a_n + b_n, \quad \forall n \geq 1.$$

Since a_n and b_n have disjoint support, we find that

$$\int_{\mathbb{R}^d} |\varphi_n|^2 = \int_{\mathbb{R}^d} |a_n|^2 + \int_{\mathbb{R}^d} |b_n|^2 = 1.$$

On the other hand, we can show that

$$\mathcal{E}_{\rm H}^V(\varphi_n) = \mathcal{E}_{\rm H}^V(a_n) + \mathcal{E}_{\rm H}^0(b_n) + o(1)_{n\to\infty}.$$

This part is similar to the Step "Splitting of energy" below. Thus by the variational principle we have the binding inequality Therefore,

$$e_{\rm H}^V(1) \leq \lim_{n\to\infty} \mathcal{E}_{\rm H}^V(\varphi_n) \leq \lim_{n\to\infty} \Big(\mathcal{E}_{\rm H}^V(a_n) + \mathcal{E}_{\rm H}^0(b_n)\Big) = e_{\rm H}^V(\lambda) + e_{\rm H}^0(1-\lambda).$$

Step 3 (Minimizing sequence). Let $\{u_n\}_{n\geq 1} \subset H^1(\mathbb{R}^d)$ be a minimizing sequence for $e_{\rm H}^V(1)$, namely

$$\|u_n\|_{L^2(\mathbb{R}^d)} = 1, \quad \mathcal{E}_{\rm H}^V(u_n) \to e_{\rm H}^V(1).$$

From the lower bound

$$\mathcal{E}_{\rm H}^V(u_n) \geq \frac{1}{2}\|\nabla u_n\|_{L^2}^2 - C$$

we find that $\{u_n\}$ is bounded in $H^1(\mathbb{R}^d)$. By the Banach-Alaoglu theorem, up to a subsequence, we can assume that $u_n \rightharpoonup u_0$ weakly in $H^1(\mathbb{R}^d)$.

Step 4 (Splitting of mass). Since $u_n \rightharpoonup u_0$ weakly in $L^2(\mathbb{R}^d)$, Fatou's lemma tells us

$$\lambda := \int_{\mathbb{R}^d} |u_0|^2 \leq \liminf_{n\to\infty} \int_{\mathbb{R}^d} |u_n|^2 = 1.$$

Moreover, if we denote

$$v_n := u_n - u_0,$$

then

$$\int_{\mathbb{R}^d} |v_n|^2 = \|u_n - u_0\|_{L^2}^2 = \|u_n\|^2 + \|u_0\|^2 - 2\Re\langle u_n, u_0\rangle \to 1 + \lambda - 2\lambda = 1 - \lambda.$$

Step 5 (Splitting of energy). We prove that

$$\lim_{n\to\infty} \Big(\mathcal{E}_{\mathrm{H}}^V(u_n) - \mathcal{E}_{\mathrm{H}}^V(u_0) - \mathcal{E}_{\mathrm{H}}^0(v_n) \Big) = 0.$$

For the kinetic energy, since $v_n = u_n - u_0 \rightharpoonup 0$ weakly in $H^1(\mathbb{R}^d)$, we have

$$\|\nabla u_n\|_{L^2}^2 - \|\nabla u_0\|_{L^2}^2 + \|\nabla v_n\|_{L^2}^2 = 2\Re\langle \nabla u_0, \nabla v_n\rangle \to 0.$$

For the external potential energy,

$$\begin{aligned}
\Big| \int_{\mathbb{R}^d} V|u_n|^2 - \int_{\mathbb{R}^d} V|u_0|^2 \Big| &\le \int_{\mathbb{R}^d} |V| \Big| |u_0 + v_n|^2 - |u_0|^2 \Big| \\
&= \int_{\mathbb{R}^d} |V| \Big(|v_n|^2 + 2|v_n||u_0| \Big) \\
&\le \int_{\mathbb{R}^d} |V||v_n|^2 + 2\sqrt{\int_{\mathbb{R}^d} |V||v_n|^2}\sqrt{\int_{\mathbb{R}^d} |V||u_0|^2} \to 0.
\end{aligned}$$

Here we used that $\int |V||u_0|^2$ is finite because $u_0 \in H^1(\mathbb{R}^d)$, and $\int |V||v_n|^2 \to 0$ because $v_n \rightharpoonup 0$ in $H^1(\mathbb{R}^d)$ (see a previous exercise).

For the interaction energy, we have

$$\begin{aligned}
&\Big| \int_{\mathbb{R}^d\times\mathbb{R}^d} \Big[|u_n(x)|^2|u_n(y)|^2 - |u_0(x)|^2|u_0(y)|^2 - |v_n(x)|^2|v_n(y)|^2 \Big] w(x-y)\mathrm{d}x\mathrm{d}y \Big| \\
&\le \Big| \int_{\mathbb{R}^d\times\mathbb{R}^d} \Big| |u_n(x)|^2|u_n(y)|^2 - |u_0(x)|^2|u_0(y)|^2 - |v_n(x)|^2|v_n(y)|^2 \Big| |w(x-y)|\mathrm{d}x\mathrm{d}y.
\end{aligned}$$

Writing $u_n = u_0 + v_n$ and expanding the difference

$$|u_n(x)|^2|u_n(y)|^2 - |u_0(x)|^2|u_0(y)|^2 - |v_n(x)|^2|v_n(y)|^2$$

we find several terms (whose absolute values) like

$$|v_n(x)||f_n(x)||u_0(y)||g_n(y)|, \quad |v_n(x)||u_0(x)||f_n(y)||g_n(y)|$$

where the functions f_n, g_n are bounded in $H^1(\mathbb{R}^d)$. By the Cauchy-Schwarz inequality, we can bound

$$\int_{\mathbb{R}^d\times\mathbb{R}^d} |v_n(x)||f_n(x)||u_0(y)||g_n(y)||w(x-y)|\mathrm{d}x\mathrm{d}y$$
$$\le \Big(\int_{\mathbb{R}^d\times\mathbb{R}^d} |v_n(x)|^2|u_0(y)|^2|w(x-y)|\mathrm{d}x\mathrm{d}y\Big)^{1/2}\Big(\int_{\mathbb{R}^d\times\mathbb{R}^d} |f_n(x)|^2|g_n(y)|^2|w(x-y)|\mathrm{d}x\mathrm{d}y\Big)^{1/2} \to 0.$$

Here we used

$$\int_{\mathbb{R}^d\times\mathbb{R}^d} |f_n(x)|^2|g_n(y)|^2|w(x-y)|\mathrm{d}x\mathrm{d}y \le C$$

because f_n, g_n are bounded in $H^1(\mathbb{R}^d)$ (the interaction energy is bounded by the kinetic energy by Step 1) and

$$\int_{\mathbb{R}^d\times\mathbb{R}^d} |v_n(x)|^2|u_0(y)|^2|w(x-y)|\mathrm{d}x\mathrm{d}y \to 0$$

because $v_n \rightharpoonup 0$ weakly in $H^1(\mathbb{R}^d)$ and $u_0 \in H^1(\mathbb{R}^d)$ (see a previous exercise). Moreover, by the Cauchy-Schwarz inequality again

$$\int_{\mathbb{R}^d\times\mathbb{R}^d} |v_n(x)||u_0(x)||f_n(y)||g_n(y)||w(x-y)|\mathrm{d}x\mathrm{d}y$$
$$\le \Big(\int_{\mathbb{R}^d\times\mathbb{R}^d} |v_n(x)||u_0(x)||f_n(y)|^2|w(x-y)|\mathrm{d}x\mathrm{d}y\Big)^{1/2}$$
$$\times \Big(\int_{\mathbb{R}^d\times\mathbb{R}^d} |v_n(x)||u_0(x)||g_n(y)|^2|w(x-y)|\mathrm{d}x\mathrm{d}y\Big)^{1/2} \to 0.$$

Here we used that f_n, g_n are bounded in $H^1(\mathbb{R}^d)$ and $|v_n u_0|^{1/2} \to 0$ strongly in $L^2(\mathbb{R}^d)$ (see an exercise below). Thus in summary, for the interaction energy we obtain

$$\Big|\int_{\mathbb{R}^d\times\mathbb{R}^d} \Big[|u_n(x)|^2|u_n(y)|^2 - |u_0(x)|^2|u_0(y)|^2 - |v_n(x)|^2|v_n(y)|^2\Big] w(x-y)\mathrm{d}x\mathrm{d}y\Big| \to 0.$$

We conclude that

$$\lim_{n\to\infty}\Big(\mathcal{E}_{\mathrm{H}}^V(u_n) - \mathcal{E}_{\mathrm{H}}^V(u_0) - \mathcal{E}_{\mathrm{H}}^0(v_n)\Big) = 0.$$

Step 6 (Conclusion from binding inequality). From the above estimates we find that

$$e_{\mathrm{H}}^V(1) = \lim_{n\to\infty}\mathcal{E}_{\mathrm{H}}^V(u_n) = \mathcal{E}_{\mathrm{H}}^V(u_0) + \lim_{n\to\infty}\mathcal{E}_{\mathrm{H}}^0(v_n) \ge e_{\mathrm{H}}^V(\lambda) + e_{\mathrm{H}}^0(1-\lambda).$$

On the other hand, we have the binding inequality $e_{\mathrm{H}}^V(1) \le e_{\mathrm{H}}^V(\lambda) + e_{\mathrm{H}}^0(1-\lambda)$. Thus here we must have that

$$\lim_{n\to\infty} \mathcal{E}_{\rm H}^0(v_n) = e_{\rm H}^0(1-\lambda),$$

namely v_n is a minimizing sequence for $e_{\rm H}^0(1-\lambda)$, and

$$\mathcal{E}_{\rm H}^V(u_0) = e_{\rm H}^V(\lambda),$$

namely u_0 is a minimizer for $e_{\rm H}^V(\lambda)$. In principle we only know that $\lambda \le 1$.

Step 7 (Conclusion from strict binding inequality). If $\lambda < 1$, we have

$$e_{\rm H}^V(1) = e_{\rm H}^V(\lambda) + e_{\rm H}^0(1-\lambda)$$

(and $e_{\rm H}^V(\lambda)$ has a minimizer). This violates the strict binding inequality. Putting differently, if the strict binding inequality holds, then $\lambda = 1$, and $e_{\rm H}^V(1)$ has a miminizer. *q.e.d.*

Exercise. *Assume that $f_n \rightharpoonup 0$ in $H^1(\mathbb{R}^d)$ and let $g \in H^1(\mathbb{R}^d)$. Prove that $|f_n g|^{1/2} \to 0$ strongly in $L^p(\mathbb{R}^d)$ for any $2 \le p < 2^*$ (with $2^* = \infty$ if $d \ge 2$ and $2^* = \frac{2d}{d-2}$ if $d \ge 3$).*

Exercise. *Consider the Hartree functional*

$$\mathcal{E}_{\rm H}^V(u) := \int_{\mathbb{R}^d} \Big(|\nabla u(x)|^2 + V(x)|u(x)|^2 \Big) {\rm d}x + \frac{1}{2} \iint_{\mathbb{R}^d\times\mathbb{R}^d} |u(x)|^2 |u(y)|^2 w(x-y) {\rm d}x{\rm d}y$$

with $V, w \in L^p(\mathbb{R}^d) + L^q(\mathbb{R}^d)$ for some $\max(d/2,1) < p, q < \infty$. Let $\lambda \in [0,1]$ and define the Hartree energy

$$e_{\rm H}^V(\lambda) := \inf\Big\{ \mathcal{E}_{\rm H}(u) \,|\, u \in H^1(\mathbb{R}^d), \|u\|_{L^2(\mathbb{R}^d)}^2 = \lambda \Big\}.$$

1. *Prove that*

$$e_{\rm H}^V(\lambda) \le e_{\rm H}^0(\lambda) \le 0.$$

2. *Deduce that if $V, w \ge 0$, then*

$$e_{\rm H}^V(\lambda) = e_{\rm H}^0(\lambda) = 0.$$

Here is an example of the application of the previous theorem.

Theorem (Existence of minimizers for bosonic atoms)**.** *Consider the Hartree functional for atoms*

$$\mathcal{E}_{\rm H}(u) := \int_{\mathbb{R}^3}\Big(|\nabla u(x)|^2 - \frac{Z}{|x|}|u(x)|^2\Big){\rm d}x + \frac{1}{2}\iint_{\mathbb{R}^3\times\mathbb{R}^3}\frac{|u(x)|^2|u(y)|^2}{|x-y|}{\rm d}x{\rm d}y$$

with $Z>0$. Then for any $0\le\lambda\le Z$, the variational problem

$$E(Z,\lambda) = \inf\Big\{\mathcal{E}_{\rm H}(u)\,|\,u\in H^1(\mathbb{R}^3), \int_{\mathbb{R}^3}|u|^2=\lambda\Big\}$$

has a minimizer.

Proof. Since the Coulomb potential $|x|^{-1}$ belongs to $L^{3-\varepsilon}(\mathbb{R}^3)+L^{3+\varepsilon}(\mathbb{R}^3)$, we can apply the previous theorem. Here we are considering a positive interaction potential. Therefore, the binding inequality becomes

$$E(Z,\lambda)\le E(Z,\lambda'),\quad \forall 0\le\lambda'\le\lambda$$

and it suffices to show that when $\lambda\le Z$ we have the strict binding inequality

$$E(Z,\lambda)< E(Z,\lambda'),\quad \forall 0\le\lambda'<\lambda$$

when $E(Z,\lambda')$ has a minimizer. It suffices to construct a trial state u such that

$$\int_{\mathbb{R}^3}|u|^2\le\lambda,\quad \mathcal{E}_{\rm H}(u)<E(Z,\lambda').$$

In fact, from this trial state, by the the monotonicity of the ground state energy in the mass and the variational principle we get

$$E(Z,\lambda)\le E(Z,\|u\|_{L^2}^2)\le\mathcal{E}_{\rm H}(u)<E(Z,\lambda').$$

We construct the trial state by following the idea of Zhilin's theorem.

Step 1 (A localized function). We prove that for $R>0$ large there exists a function $u_R\in H^1(\mathbb{R}^3)$ such that

$${\rm supp}(u_R)\subset\{|x|\le R\},\quad \int|u_R|^2\le\lambda',\quad \mathcal{E}_{\rm H}(u_R)\le E(Z,\lambda')+o(R^{-1})_{R\to\infty}.$$

Let u_0 be a minimizer for $E(Z,\lambda')$. Let $\chi,\eta:\mathbb{R}^3\to[0,1]$ be smooth functions such that $\chi^2+\eta^2=1$, $\chi(x)=1$ if $|x|<1/2$ and $\chi(x)=0$ if $|x|\ge 1$. Define

$$\chi_R(x)=\chi(x/R),\quad u_R=\chi_R u_0.$$

Clearly we have

$$\operatorname{supp}(u_R)\subset\{|x|\le R\},\quad \int |u_R|^2\le\int|u_0|^2=\lambda'.$$

It remains to estimate the energy difference $\mathcal{E}_{\rm H}(u_R)-\mathcal{E}_{\rm H}(u_0)$. For the kinetic energy, by using the partition of unity

$$\chi_R^2+\eta_R^2=1,\quad \chi_R(x)=\chi(x/R),$$

and the IMS formula we can estimate

$$\begin{aligned}\int|\nabla u_R|^2-\int|\nabla u_0|^2&\le\int|\nabla(\chi_R u_0)|^2+\int|\nabla(\eta_R u_0)|^2-\int|\nabla u_0|^2\\&=\int_{\mathbb{R}^3}(|\nabla\chi_R|^2+|\nabla\eta_R|^2)|u_0|^2\le O(R^{-2}).\end{aligned}$$

For the potential energy, we have

$$-\int\frac{Z}{|x|}\Big[|u_R|^2-|u_0|^2\Big]=\int\frac{Z}{|x|}|\eta_R u_0|^2\le\frac{2Z}{R}\int_{|x|\ge R/2}|u_0|^2=o(R^{-1}).$$

For the interaction energy, since the interaction potential is positive, we simply use to point-wise estimate $|u_R(x)|\le|u_0(x)|$ to get

$$\frac12\iint_{\mathbb{R}^3\times\mathbb{R}^3}\frac{|u_R(x)|^2|u_R(y)|^2}{|x-y|}\mathrm{d}x\mathrm{d}y-\frac12\iint_{\mathbb{R}^3\times\mathbb{R}^3}\frac{|u_0(x)|^2|u_0(y)|^2}{|x-y|}\mathrm{d}x\mathrm{d}y\le 0.$$

Thus we have

$$\mathcal{E}_{\rm H}(u_R)\le\mathcal{E}_{\rm H}(u_0)+o(R^{-1})=E(Z,\lambda')+o(R^{-1}).$$

Step 2 (A function " at infinity"). Take a smooth function $v:\mathbb{R}^3\to\mathbb{R}$ with

$$\operatorname{supp} v\subset\{x\in\mathbb{R}^3:1<|x|<2\},\quad\int_{\mathbb{R}^d}|v|^2=\varepsilon.$$

For any $R>0$ we choose

$$v_R(x)=\frac{1}{R^{3/2}}v\Big(\frac{x}{R}\Big).$$

Then

$$\operatorname{supp} v_R \subset \{x \in \mathbb{R}^3 : R \le |x| \le 2R\}, \qquad \int_{\mathbb{R}^3} |v_R|^2 = \varepsilon.$$

Step 3 (The trial state). We choose the trial state

$$\varphi_R = u_R + v_R \in H^1(\mathbb{R}^d).$$

Since u_R and v_R have disjoint supports, we have

$$\|\varphi_R\|_{L^2}^2 = \|u_R + v_R\|_{L^2}^2 = \|u_R\|_{L^2}^2 + \|v_R\|_{L^2}^2 \le \lambda' + \varepsilon.$$

We can choose $\varepsilon > 0$ small such that $\lambda' + \varepsilon < \lambda$.

Step 4 (Strict binding inequality). Now we estimate $\mathcal{E}_{\rm H}(\varphi_R) - \mathcal{E}_{\rm H}(u_R)$. For the kinetic energy, since u_R and v_R have disjoint supports

$$\|\nabla\varphi_R\|_{L^2}^2 - \|\nabla u_R\|_{L^2}^2 = \|\nabla v_R\|_{L^2}^2 = O(R^{-2}).$$

For the potential energy,

$$-\int_{\mathbb{R}^3} \frac{Z}{|x|}\Big[|\varphi_R|^2 - |u_R|^2\Big] = -\int_{\mathbb{R}^3} \frac{Z}{|x|}|v_R|^2 = -\frac{Z}{R}\int_{\mathbb{R}^3} \frac{1}{|x|}|v|^2.$$

For the interaction energy, using Newton's theorem (v_R is radial) we can bound

$$\begin{aligned}
&\frac{1}{2}\iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|\varphi_R(x)|^2|\varphi_R(y)|^2 - |u_R(x)|^2|u_R(y)|^2}{|x-y|}\\
&= \frac{1}{2}\iint \frac{(|u_R(x)|^2 + |v_R(x)|^2)(|u_R(y)|^2 + |v_R(y)|^2) - |u_R(x)|^2|u_R(y)|^2}{|x-y|}\\
&= \frac{1}{2}\iint \frac{2|u_R(x)|^2|v_R(y)|^2 + |v_R(x)|^2|v_R(y)|^2}{|x-y|}\\
&= \frac{1}{2}\iint \frac{2|u_R(x)|^2|v_R(y)|^2 + |v_R(x)|^2|v_R(y)|^2}{\max(|x|,|y|)}\\
&\le \frac{1}{2}\iint \frac{2|u_R(x)|^2|v_R(y)|^2 + |v_R(x)|^2|v_R(y)|^2}{|y|}\\
&= (\lambda' + \varepsilon/2)\int \frac{|v_R(y)|^2}{|y|} = \frac{\lambda' + \varepsilon/2}{R}\int \frac{|v(y)|^2}{|y|}.
\end{aligned}$$

Thus in summary

$$\mathcal{E}_{\mathrm{H}}(\varphi_R) - \mathcal{E}_{\mathrm{H}}(u_R) \leq \frac{\lambda' + \varepsilon/2 - Z}{R} \int \frac{|v(y)|^2}{|y|} + O(R^{-2}).$$

Moreover, from the choice of u_R we have

$$\mathcal{E}_{\mathrm{H}}(u_R) \leq e_{\mathrm{H}}(\lambda') + o(R^{-1}).$$

Thus

$$\mathcal{E}_{\mathrm{H}}(\varphi_R) \leq e_{\mathrm{H}}(\lambda') + \leq \frac{\lambda' + \varepsilon/2 - Z}{R} \int \frac{|v(y)|^2}{|y|} + o(R^{-1}).$$

Here we are choosing $\lambda' + \varepsilon \leq \lambda \leq Z$, therefore

$$\lambda' + \varepsilon/2 - Z < 0.$$

Thus if we take R large enough, then

$$\mathcal{E}_{\mathrm{H}}(\varphi_R) < e_{\mathrm{H}}(\lambda')$$

which completes the proof. *q.e.d.*

Exercise. *Consider the Hartree functional*

$$\mathcal{E}_{\mathrm{H}}(u) := \int_{\mathbb{R}^3} \Big(|\nabla u(x)|^2 - Z \frac{|u(x)|^2}{|x|} \Big) \mathrm{d}x + \frac{1}{2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{|u(x)|^2 |u(y)|^2}{|x-y|^s} \mathrm{d}x \mathrm{d}y$$

with parameters $Z > 0$ and $1 < s < 2$. Prove that the minimization problem

$$e_{\mathrm{H}} := \inf \Big\{ \mathcal{E}_{\mathrm{H}}(u) \,|\, u \in H^1(\mathbb{R}^d), \|u\|_{L^2(\mathbb{R}^d)} = 1 \Big\}$$

has a minimizer.

3.3 Existence of minimizers: translation-invariant case

Now we consider the special case when the external potential is zero. This corresponds to the "problem at infinity". In this case, the Hartree functional

$$\mathcal{E}_{\rm H}^{0}(u) := \int_{\mathbb{R}^d} |\nabla u(x)|^2 {\rm d}x + \frac{1}{2}\iint_{\mathbb{R}^d\times\mathbb{R}^d} |u(x)|^2|u(y)|^2 w(x-y){\rm d}x{\rm d}y$$

is **translation-invariant**, namely

$$\mathcal{E}_{\rm H}^{0}(u) = \mathcal{E}_{\rm H}^{0}(u(\cdot - y)), \quad \forall u \in H^1(\mathbb{R}^d), \quad \forall y \in \mathbb{R}^d.$$

We know that if $w \geq 0$ (and w vanishes at infinity), then the corresponding energy

$$e_{\rm H}^{0}(\lambda) := \inf\{\mathcal{E}_{\rm H}^{0}(u) \,|\, u \in H^1(\mathbb{R}^d), \|u\|_{L^2}^2 = \lambda\}$$

is simply zero. However, if $w \leq 0$ (or if w has a non-trivial negative part), then in principle the energy $e_{\rm H}^{0}(\lambda)$ can be negative. Thus even if we start with a general (non-zero) external potential V, understanding the problem at infinity is still very helpful to justify the binding inequality

$$\mathcal{E}_{\rm H}^{V}(1) < \mathcal{E}_{\rm H}^{V}(\lambda) + \mathcal{E}_{\rm H}^{0}(1-\lambda), \quad \forall 0 \leq \lambda < 1.$$

On the other hand, the method in the previous section is not enough to deal with the translation-invariant case, because the binding inequality

$$\mathcal{E}_{\rm H}^{V}(1) < \mathcal{E}_{\rm H}^{V}(\lambda) + \mathcal{E}_{\rm H}^{0}(1-\lambda), \quad \forall 0 \leq \lambda < 1.$$

cannot hold true with $V \equiv 0$ (just take $\lambda = 0$). Therefore, we will need the following result.

Theorem (Existence of Hartree minimizers: translation-invariant case)**.** *Consider the Hartree functional*

$$\mathcal{E}_{\rm H}^{0}(u) := \int_{\mathbb{R}^d} |\nabla u(x)|^2 {\rm d}x + \frac{1}{2}\iint_{\mathbb{R}^d\times\mathbb{R}^d} |u(x)|^2|u(y)|^2 w(x-y){\rm d}x{\rm d}y$$

with $w \in L^p(\mathbb{R}^d) + L^p(\mathbb{R}^d)$, $\max(d/2, 1) < p, q < \infty$. *For any* $\lambda \in [0,1]$ *define*

$$e_{\rm H}^{0}(\lambda) := \inf\Big\{\mathcal{E}_{\rm H}^{0}(u) : u \in H^1(\mathbb{R}^d), \|u\|_{L^2(\mathbb{R}^d)}^2 = \lambda\Big\}.$$

Then we always have the binding inequality

$$e^0_{\rm H}(\lambda) \le e^0_{\rm H}(\lambda') + e^0_{\rm H}(\lambda-\lambda'), \quad \forall 0<\lambda'<\lambda.$$

Moreover, if we have the **strict binding inequality**

$$e^0_{\rm H}(\lambda) < e^0_{\rm H}(\lambda') + e^0_{\rm H}(\lambda-\lambda'), \quad \forall 0<\lambda'<\lambda,$$

then $e^0_{\rm H}(\lambda)$ has a minimizer. In fact, for the existence of minimizers for $e^0_{\rm H}(\lambda)$, we only need the strict binding inequality when both $e^0_{\rm H}(\lambda')$ and $e^0_{\rm H}(\lambda-\lambda')$ have minimizers.

Remarks:

- Note that in the above strict binding inequality we do not include the case $\lambda'=0$ (and the case $\lambda'=\lambda$). This is the main difference to the previous section .
- Since $e^0_{\rm H}(\lambda')\le 0$ for all λ' (see a previous exercise), the strict binding inequality in particular implies the non-vanishing condition $e^0_{\rm H}(\lambda)<0$.

The main difficulty in the proof of the above Theorem is as follows: if u_0 is a minimizer for $e^0_{\rm H}(\lambda)$, then

$$u_n(x)=u_0(x-y_n), \quad y_n\in\mathbb{R}^d$$

are also minimizers for $e^0_{\rm H}(\lambda)$. On the other hand, if $\lim_{n\to\infty}|y_n|=+\infty$, then $u_n\rightharpoonup 0$ weakly in $H^1(\mathbb{R}^d)$. Similarly, there are several minimizing sequences for $e^0_{\rm H}(\lambda)$ that converge weakly to 0. Thus to apply the method of calculus of variations, we have to modify minimizing sequences using appropriate translations.

Exercise. *Assume that $u_n\to u_0$ strongly in $L^2(\mathbb{R}^d)$. Let $\{y_n\}_{n=1}^\infty\subset\mathbb{R}^d$ such that $|y_n|\to+\infty$ and denote*

$$v_n(x):=u_n(x-y_n), \quad \forall x\in\mathbb{R}^d, \quad \forall n\in\mathbb{N}.$$

Prove that $v_n\rightharpoonup 0$ weakly in $L^2(\mathbb{R}^d)$.

The following key lemma provides a proper understanding of the **vanishing case** in the translation-invariant setting, namely the situation when we have the weak convergence to 0 up to all translations.

Lemma (Concentration–Compactness Lemma.). *Let $\{u_n\}_{n\ge1}$ be a bounded sequence in $H^1(\mathbb{R}^d)$. Then there are two alternatives:*

- **Vanishing case:** *$u_n \to 0$ strongly in $L^r(\mathbb{R}^d)$ for all $2 < r < 2^*$, where $2^* = \infty$ if $d \le 2$ and $2^* = 2d/(d-2)$ if $d \ge 3$.*
- **Non-vanishing case:** *There exist a subsequence $\{u_{n_k}\}_{k\ge1}$ and a sequence $\{y_k\} \subset \mathbb{R}^d$ such that $v_k := u_{n_k}(\cdot - y_k)$ converges weakly to a function $v_0 \not\equiv 0$ in $H^1(\mathbb{R}^d)$.*

Proof. We define **"the largest mass that stays in a bounded region"**

$$\mathfrak{M}(\{u_n\}) := \lim_{R\to\infty} \limsup_{n\to\infty} \sup_{y\in\mathbb{R}^d} \int_{|x-y|\le R} |u_n(x)|^2 \mathrm{d}x.$$

There are two possibilities.

Case 1: Non-vanishing: $\mathfrak{M}(\{u_n\}) > 0$. Then by the definition, there exists $R > 0$ such that

$$\limsup_{n\to\infty} \sup_{y\in\mathbb{R}^d} \int_{|x-y|\le R} |u_n(x)|^2 \mathrm{d}x > 0.$$

Thus there exists a subsequence $\{u_{n_k}\}$, a sequence $\{y_k\} \subset \mathbb{R}^d$ and $\varepsilon > 0$ such that

$$\int_{|x-y_k|\le R} |u_{n_k}(x)|^2 \mathrm{d}x \ge \varepsilon > 0, \quad \forall k \ge 1.$$

Define $v_k := u_{n_k}(x - y_k)$. Then the above lower bound can be rewritten as

$$\int_{|x|\le R} |v_k(x)|^2 \mathrm{d}x \ge \varepsilon > 0, \quad \forall k \ge 1.$$

On the other hand, $\|v_k\|_{H^1} = \|u_{n_k}\|_{H^1}$ is bounded. Therefore, up to a subsequence we can assume that $v_k \rightharpoonup v_0$ weakly in $H^1(\mathbb{R}^d)$. By the Sobolev's embedding theorem we find that

$$\int_{|x|\le R} |v_0(x)|^2 \mathrm{d}x = \lim_{k\to\infty} \int_{|x|\le R} |v_k(x)|^2 \mathrm{d}x \ge \varepsilon.$$

Thus $v_0 \not\equiv 0$, as desired.

Case 2: Vanishing: $\mathfrak{M}(\{u_n\}) = 0$. Then for all $R > 0$ we have

$$\lim_{n\to\infty} \sup_{y\in\mathbb{R}^d} \int_{|x-y|\leq R} |u_n(x)|^2 \mathrm{d}x = 0.$$

Fix $R > 0$ sufficiently large. We can write the space $\mathbb{R}^d$ as a union of finite balls

$$\mathbb{R}^d = \bigcup_{z\in\mathbb{Z}^d} B(z, R/2).$$

Let $\chi : \mathbb{R}^d \to [0,1]$ be a smooth function such that $\chi(x) = 1$ if $|x| \leq R/2$ and $\chi(x) = 0$ if $|x| \geq R$. Define $\chi_z(x) = \chi(x-z)$. Then

$$1 \leq \sum_{z\in\mathbb{R}^d} \chi_z(x)^s \leq C, \quad \sum_{z\in\mathbb{R}^d} |\nabla\chi_z(x)|^2 \leq C, \quad \forall x \in \mathbb{R}^d, \quad \forall s \in (0,\infty).$$

For any $z \in \mathbb{R}^d$, by Hölder inequality we have

$$\int_{\mathbb{R}^d} |\chi_z u_n|^r \leq \Big(\int_{\mathbb{R}^d} |\chi_z u_n|^2\Big)^\theta \Big(\int_{\mathbb{R}^d} |\chi_z u_n|^q\Big)^{1-\theta}$$

for any

$$2 < r < q, \quad 0 < \theta < 1, \quad 2\theta + q(1-\theta) = r.$$

In particular, for $r > 2$ and sufficiently close to 2, we can choose

$$\theta = \frac{r}{2} - 1, \quad q = \frac{4}{4-r} < 2^*, \quad \text{such that} \quad q(1-\theta) = 2.$$

The conditions $q < 2^*$ and $q(1-\theta) = 2$ allow us to use Sobolev's inequality

$$\Big(\int_{\mathbb{R}^d} |\chi_z u_n|^q\Big)^{1-\theta} = \|\chi_z u_n\|_{L^q}^2 \leq C\|\chi_z u_n\|_{H^1}^2.$$

Thus in summary, for $r > 2$ and close to 2 we have

$$\int_{\mathbb{R}^d} |\chi_z u_n|^r \leq C\Big(\int_{\mathbb{R}^d} |\chi_z u_n|^2\Big)^{r/2-1} \|\chi_z u_n\|_{H^1}^2.$$

Summing over $z \in \mathbb{R}^d$ we obtain

$$\int_{\mathbb{R}^d} |u_n|^r \leq \sum_{z\in\mathbb{R}^d} \int_{\mathbb{R}^d} |\chi_z u_n|^r \leq C\Big[\sup_{y\in\mathbb{Z}^d} \int_{\mathbb{R}^d} |\chi_y u_n|^2\Big]^{r/2-1} \sum_{z\in\mathbb{R}^d} \|\chi_z u_n\|_{H^1(\mathbb{R}^d)}^2$$

$$\le C\Big(\sup_{y\in\mathbb{R}^d}\int_{|x-y|\le R}|u_n(x)|^2\mathrm{d}x\Big)^{r/2-1}\|u_n\|^2_{H^1(\mathbb{R}^d)}\to 0.$$

Here we have used $\sum_{z\in\mathbb{R}^d}\|\chi_z u_n\|^2_{H^1}\le C\|u_n\|^2_{H^1}$ (see an exercise below), together with the fact that $\|u_n\|_{H^1(\mathbb{R}^d)}$ is bounded and the vanishing condition. Thus $u_n\to 0$ strongly in $L^r(\mathbb{R}^d)$ with $r>2$ and close to 2. Since $\{u_n\}$ is bounded in $H^1(\mathbb{R}^d)$, by interpolation (Sobolev's and Hölder's inequalities) we conclude that $u_n\to 0$ strongly in $L^r(\mathbb{R}^d)$ for any $2<r<2^*$. *q.e.d.*

Exercise. *Let $\{u_n\}_{n\ge1}$ be a bounded sequence in $H^1(\mathbb{R}^d)$. Define*

$$\mathfrak{M}(\{u_n\}) := \lim_{R\to\infty}\limsup_{n\to\infty}\sup_{y\in\mathbb{R}^d}\int_{|x-y|\le R}|u_n(x)|^2\mathrm{d}x$$

and

$$\mathfrak{M}'(\{u_n\}) := \sup\{\|v\|^2_{L^2(\mathbb{R}^d)}\,|\,\exists \text{ a subsequence } u_{n_k}(\cdot-y_k)\rightharpoonup v \text{ weakly in } H^1(\mathbb{R}^d)\}.$$

(Here $\{u_{n_k}\}$ is a subsequence of $\{u_n\}$ and the sequence $\{y_k\}\subset\mathbb{R}^d$ can be chosen arbitrarily). Prove that

$$\mathfrak{M}(\{u_n\})=\mathfrak{M}'(\{u_n\}).$$

Exercise. *Let $\{\chi_n\}_{n\ge1}$ be a sequence of smooth functions $\chi_n:\mathbb{R}^d\to[0,1]$ satisfying*

$$\sup_{x\in\mathbb{R}^d}\sum_{n\ge1}\Big[|\chi_n(x)|^2+|\nabla_x\chi_n(x)|^2\Big]<\infty.$$

Prove that

$$\sum_{n\ge1}\|\chi_n u\|^2_{H^1}\le C\|u\|^2_{H^1(\mathbb{R}^d)},\quad \forall u\in H^1(\mathbb{R}^d).$$

The constant $C>0$ is dependent on $\{\chi_n\}_{n\ge1}$, but independent of u.

Proof of the existence theorem. The finiteness of $e^0_{\mathrm{H}}(\lambda)$ and the binding inequality

$$e^0_{\mathrm{H}}(\lambda)\le e^0_{\mathrm{H}}(\lambda')+e^0_{\mathrm{H}}(\lambda-\lambda'),\quad \forall 0<\lambda'<\lambda$$

have been proved before. Thus it remains to prove the existence of minimizers under the strict binding inequality

$$e^0_{\rm H}(\lambda) < e^0_{\rm H}(\lambda') + e^0_{\rm H}(\lambda - \lambda'), \quad \forall 0 < \lambda' < \lambda.$$

From the lower bound

$$\mathcal{E}^0_{\rm H}(u) \geq \frac{1}{2}\int_{\mathbb{R}^d} |\nabla u|^2 - C$$

we find that any minimizing sequence for $e^0_{\rm H}(\lambda)$ is bounded in $H^1(\mathbb{R}^d)$. Thus by the concentration-compactness lemma, there are two possibilities: vanishing case and non-vanishing case.

Vanishing case: $u_n \to 0$ strongly in $L^r(\mathbb{R}^d)$ for all $2 < r < 2^*$. In this case, using $w \in L^p(\mathbb{R}^d) + L^q(\mathbb{R}^d)$ with $p, q > \max(d/2, 1)$ we find that

$$\iint_{\mathbb{R}^d \times \mathbb{R}^d} |u_n(x)|^2 |u_n(y)|^2 w(x-y) {\rm d}x{\rm d}y \to 0.$$

In fact, if $w \in L^p(\mathbb{R}^d)$ for example, then by Hölder and Young inequalities

$$\iint_{\mathbb{R}^d \times \mathbb{R}^d} |u_n(x)|^2 |u_n(y)|^2 |w(x-y)| {\rm d}x{\rm d}y \leq \||u_n|^2\|_{L^{p'}} \|w * |u_n|^2\|_{L^p} \leq \|u_n\|^2_{L^{2p'}} \|w\|_{L^p} \|u_n\|^2_{L^2} \to 0.$$

Here

$$\frac{1}{p} + \frac{1}{p'} = 1$$

and the condition $p > \max(d/2, 1)$ implies that $2 < p' < 2^*$. Consequently, we find that

$$e^0_{\rm H}(\lambda) = \lim_{n\to\infty} \mathcal{E}^0_{\rm H}(u_n) \geq 0.$$

However, it contradicts with the strict binding inequality (which particularly implies that $e^0_{\rm H}(\lambda) < 0$).

Non-vanishing case: Up to subsequences and translations, we can assume that $u_n \rightharpoonup u_0$ weakly in $H^1(\mathbb{R}^d)$ with $u_0 \not\equiv 0$. As proved in the previous section , we can split the energy

$$\lim_{n\to\infty} \Big(\mathcal{E}^0_{\rm H}(u_n) - \mathcal{E}^0_{\rm H}(u_0) - \mathcal{E}^0_{\rm H}(u_n - u_0) \Big) = 0.$$

Denote $\lambda' := \|u_0\|^2_{L^2} > 0$. Then

$$\|u_n - u_0\|_{L^2} = \|u_n\|^2_{L^2} + \|u_0\|^2_{L^2} - 2\Re\langle u_n, u_0\rangle \to \lambda + \lambda' - 2\lambda' = \lambda - \lambda'.$$

Thus by the variational principle we have

$$e_{\rm H}^0(\lambda) = \lim_{n\to\infty} \mathcal{E}_{\rm H}^0(u_n) \geq \mathcal{E}_{\rm H}^0(u_0) + \lim_{n\to\infty} \mathcal{E}_{\rm H}^0(u_n - u_0) \geq e_{\rm H}^0(\lambda') + e_{\rm H}^0(\lambda-\lambda').$$

In comparison to the binding inequality

$$e_{\rm H}^0(\lambda) \leq e_{\rm H}^0(\lambda') + e_{\rm H}^0(\lambda-\lambda')$$

we find that $\mathcal{E}_{\rm H}^0(u_0) = e_{\rm H}^0(\lambda')$ (i.e. u_0 is a minimizer for $e_{\rm H}^0(\lambda')$).
Moreover, if the strict binding inequality holds, then we must have $\lambda' = \lambda$ (as we have known already that $\lambda' = \|u_0\|_{L^2}^2 > 0$. Thus u_0 is a minimizer for $e_{\rm H}^0(\lambda)$. *q.e.d.*

Here is an application of the above abstract theorem.

Theorem (Choquard-Pekar Problem)**.** *Consider the Hartree functional with gravitational interaction potential*

$$\mathcal{E}_{\rm H}^0(u) := \int_{\mathbb{R}^3} |\nabla u|^2 - \frac{1}{2}\iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|u(x)|^2|u(y)|^2}{|x-y|}{\rm d}x{\rm d}y.$$

Prove that for every $\lambda > 0$, the minimization problem

$$e_{\rm H}^0(\lambda) := \inf\left\{\mathcal{E}_{\rm H}^0(u)\,|\, u\in H^1(\mathbb{R}^d), \|u\|_{L^2}^2 = \lambda\right\}$$

has a minimizer.

Proof. Recall that $-|x|^{-1} \in L^{3-\varepsilon}(\mathbb{R}^3) + L^{3+\varepsilon}(\mathbb{R}^3)$. We need to check the strict binding inequality

$$e_{\rm H}^0(\lambda) < e_{\rm H}^0(\lambda') + e_{\rm H}^0(\lambda-\lambda'), \quad \forall 0<\lambda'<\lambda.$$

Step 1: We prove that $e_{\rm H}^0(\lambda) < 0$ for all $\lambda > 0$.
In fact, take $\varphi \in H^1(\mathbb{R}^3)$ with $\|\varphi\|_{L^2}^2 = \lambda$. For every $R > 0$ define

$$\varphi_R(x) = R^{-3/2}\varphi(x/R).$$

Then $\|\varphi_R\|_{L^2}^2 = \lambda$ and

$$\mathcal{E}_{\rm H}^0(\varphi_R) = \frac{1}{R^2}\|\nabla\varphi\|_{L^2}^2 - \frac{1}{2R}\iint_{\mathbb{R}^3\times\mathbb{R}^3}\frac{|\varphi(x)|^2|\varphi(y)|^2}{|x-y|}{\rm d}x{\rm d}y.$$

By taking $R > 0$ sufficiently large, we conclude by the variational principle

$$e_{\mathrm{H}}^0(\lambda) \leq \mathcal{E}_{\mathrm{H}}^0(\varphi_R) < 0.$$

Step 2: We prove that for all $\lambda > 0$, for all $0 < \theta < 1$,

$$e_{\mathrm{H}}^0(\theta\lambda) \geq \theta^2 e_{\mathrm{H}}^0(\lambda).$$

Indeed, take a minimizing sequence $\{u_n\}_{n\geq 1} \subset H^1(\mathbb{R}^d)$ for $e_{\mathrm{H}}^0(\theta\lambda)$, i.e.

$$\|u_n\|_{L^2}^2 = \theta\lambda, \quad \mathcal{E}_{\mathrm{H}}^0(u_n) \to e_{\mathrm{H}}^0(\theta\lambda).$$

Define

$$v_n = \frac{u_n}{\sqrt{\theta}}, \quad \|v_n\|_2^2 = \lambda.$$

Then by the variational principle we have

$$\begin{aligned} e_{\mathrm{H}}^0(\lambda) \leqslant \mathcal{E}_{\mathrm{H}}^0(v_n) &= \frac{1}{\theta}\|\nabla u_n\|_{L^2}^2 - \frac{1}{2\theta^2}\iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|u_n(x)|^2|u_n(y)|^2}{|x-y|}\mathrm{d}x\mathrm{d}y \\ &= \left(\frac{1}{\theta} - \frac{1}{\theta^2}\right)\|\nabla u_n\|_{L^2}^2 + \frac{1}{\theta^2}\mathcal{E}_{\mathrm{H}}^0(u_n) \\ &\leq \frac{1}{\theta^2}\mathcal{E}_{\mathrm{H}}^0(u_n) \to \frac{1}{\theta^2}e_{\mathrm{H}}^0(\theta\lambda). \end{aligned}$$

Step 3: Using the estimates in Step 1 and Step 2, for every $\lambda > \lambda' > 0$ we can bound

$$\begin{aligned} e_{\mathrm{H}}^0(\lambda') + e_{\mathrm{H}}^0(\lambda - \lambda') &= e_{\mathrm{H}}^0\Big(\frac{\lambda'}{\lambda}\lambda\Big) + e_{\mathrm{H}}^0\Big(\frac{\lambda-\lambda'}{\lambda}\lambda\Big) \\ &\geq \Big(\frac{\lambda'}{\lambda}\Big)^2 e_{\mathrm{H}}^0(\lambda) + \Big(\frac{\lambda-\lambda'}{\lambda}\Big)^2 e_{\mathrm{H}}^0(\lambda) \\ &> \Big(\frac{\lambda'}{\lambda}\Big)e_{\mathrm{H}}^0(\lambda) + \Big(\frac{\lambda-\lambda'}{\lambda}\Big)e_{\mathrm{H}}^0(\lambda) = e_0^{\mathrm{H}}(\lambda). \end{aligned}$$

Thus the strict binding inequality holds, and hence $e_0^{\mathrm{H}}(\lambda)$ has a minimizer for every $\lambda > 0$. *q.e.d.*

The above analysis can be also adapted to treat the Hartree problem with a general potential vanishing at infinity.

Exercise (Choquard-Pekar Problem with an external potential). *Consider the Hartree functional*

$$\mathcal{E}_{\mathrm{H}}^{V}(u) := \int_{\mathbb{R}^3} \Big(|\nabla u|^2 + V|u|^2\Big) - \frac{1}{2}\iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|u(x)|^2|u(y)|^2}{|x-y|}\mathrm{d}x\mathrm{d}y$$

with real-valued potentials $V, w \in L^p(\mathbb{R}^d) + L^q(\mathbb{R}^d)$, $\infty > p, q > \max(d/2, 1)$. *Assume that* $V \le 0$ *and* $V \not\equiv 0$. *Prove that for every* $\lambda > 0$ *the minimization problem*

$$e_{\mathrm{H}}^{V}(\lambda) := \inf\Big\{\mathcal{E}_{\mathrm{H}}^{V}(u) \,|\, u \in H^1(\mathbb{R}^d), \|u\|_{L^2}^2 = \lambda\Big\}$$

has a minimizer.

3.4 Hartree equation

Theorem (Hartree equation). *Consider the Hartree functional*

$$\mathcal{E}_{\mathrm{H}}^{V}(u) := \int_{\mathbb{R}^d} \Big(|\nabla u(x)|^2 + V(x)|u(x)|^2\Big)\mathrm{d}x + \frac{1}{2}\iint_{\mathbb{R}^d\times\mathbb{R}^d} |u(x)|^2|u(y)|^2 w(x-y)\mathrm{d}x\mathrm{d}y$$

with $V_-, w \in L^p(\mathbb{R}^d) + L^\infty(\mathbb{R}^d)$, $V_+ \in L^p_{\mathrm{loc}}(\mathbb{R}^d)$ *with* $p > \max(d/2, 1)$. *Assume that for some* $\lambda > 0$ *the minimization problem*

$$e_{\mathrm{H}}^{V}(\lambda) := \inf\Big\{\mathcal{E}_{\mathrm{H}}^{V}(u) : u \in H^1(\mathbb{R}^d), \|u\|_{L^2(\mathbb{R}^d)}^2 = \lambda\Big\}$$

has a minimizer u_0. *Then* u_0 *satisfies the* **Hartree equation**

$$\Big(-\Delta + V(x) + (w * |u_0|^2)(x) - \mu(\lambda)\Big)u_0(x) = 0.$$

in the **distributional sense**, *namely*

$$\int_{\mathbb{R}^d} \Big[\nabla\overline{\varphi}\cdot\nabla u_0 + V\overline{\varphi}u_0 + \overline{\varphi}(w * |u_0|^2)u_0 - \mu\overline{\varphi}u_0\Big] = 0, \quad \forall \varphi \in C_c^\infty(\mathbb{R}^d).$$

Here the constant $\mu(\lambda) \in \mathbb{R}$ *is called the* **Lagrange multiplier** *or* **chemical potential**.

Proof. Let us consider the case $\lambda = 1$ for simplicity. By the variational principle, for every

$\varphi \in C_c^\infty(\mathbb{R}^d)$ we have

$$\mathcal{E}_{\mathrm{H}}^V\Big(\frac{u_0+\varepsilon\varphi}{\|u_0+\varepsilon\varphi\|_{L^2}}\Big) \ge \mathcal{E}_{\mathrm{H}}^V(u_0)$$

for all $\varepsilon \in \mathbb{R}$ sufficiently close to 0. Therefore,

$$0 = \frac{d}{d\varepsilon}\mathcal{E}_{\mathrm{H}}^V\Big(\frac{u_0+\varepsilon\varphi}{\|u_0+\varepsilon\varphi\|_{L^2}}\Big)|_{\varepsilon=0} = 2\Re\int_{\mathbb{R}^d}\Big[\nabla\overline{\varphi}\cdot\nabla u_0 + V\overline{\varphi}u_0 + \overline{\varphi}(w*|u_0|^2)u_0 - \mu\overline{\varphi}u_0\Big]$$

with

$$\mu = \int_{\mathbb{R}^d}\Big(|\nabla u_0(x)|^2 + V(x)|u_0(x)|^2\Big)\mathrm{d}x + \iint_{\mathbb{R}^d\times\mathbb{R}^d}|u_0(x)|^2|u_0(y)|^2 w(x-y)\mathrm{d}x\mathrm{d}y.$$

Replacing φ by $\mathbf{i}\varphi$ (with $\mathbf{i}^2=-1$) we find that

$$0 = 2\Im\int_{\mathbb{R}^d}\Big[\nabla\overline{\varphi}\cdot\nabla u_0 + V\overline{\varphi}u_0 + \overline{\varphi}(w*|u_0|^2)u_0 - \mu\overline{\varphi}u_0\Big].$$

Thus for all $\varphi \in C_c^\infty(\mathbb{R}^d)$ we have

$$\int_{\mathbb{R}^d}\Big[\nabla\overline{\varphi}\cdot\nabla u_0 + V\overline{\varphi}u_0 + \overline{\varphi}(w*|u_0|^2)u_0 - \mu\overline{\varphi}u_0\Big] = 0.$$

q.e.d.

3.5 Regularity of minimizers

Theorem (Hartree equation)**.** *Assume that $u_0 \in H^1(\mathbb{R}^d)$ is a solution to the Hartree equation*

$$\Big(-\Delta + V(x) + (w*|u_0|^2)(x) - \mu\Big)u_0 = 0.$$

in the distributional sense. Assume that $\mu\in\mathbb{R}$, $V = V_1 + V_2$ and

- *$V_1, w \in L^p(\mathbb{R}^d) + L^\infty(\mathbb{R}^d)$ with $p > \max(d/2, 2)$;*
- *$0 \le V_2 \in L^\infty_{\mathrm{loc}}$ and $|\nabla V_2(x)| \le C(V_2(x)+1)$.*

Then $u_0 \in H^2(\mathbb{R}^d)$ and $-\Delta u_0$, $Vu_0 \in L^2(\mathbb{R}^d)$, $(w*|u_0|^2)u_0 \in L^2(\mathbb{R}^d)$. In particular, the Hartree equation holds in the pointwise sense.

Remark: The conditions $V_2 \ge 0$ and $|\nabla V_2(x)| \le C(V_1(x)+1)$ allow trapping potentials, e.g.

$V_2(x) \to +\infty$ as $|x| \to \infty$ and it does not grow faster than exponentially.

Proof. **Potentials vanishing at infinity.** First let us consider the case $V_2 \equiv 0$, namely $V = V_1$ vanishes at infinity. In this case, since $V \in L^p + L^\infty$ with $p > \max(d/2, 2)$, it is relatively bounded with the Laplacian with an arbitrarily relative bound, namely

$$\|V\varphi\|_{L^2} \le \varepsilon\|\Delta\varphi\|_{L^2} + C_\varepsilon\|\varphi\|_{L^2}, \quad \forall \varphi \in H^2(\mathbb{R}^d), \quad \forall \varepsilon > 0.$$

Moreover, we have $w * |u_0|^2 \in L^\infty(\mathbb{R}^d)$. Indeed, if $w \in L^p$ for example, then by Young's and Sobolev's inequality we find that

$$\|w * |u_0|^2\|_{L^\infty} \le \|w\|_{L^p}\|u_0^2\|_{L^{p'}} = \|w\|_{L^p}\|u_0\|_{L^{2p'}}^2 \le C\|w\|_{L^p}\|u_0\|_{H^1}^2.$$

Here $1/p + 1/p' = 1$ and the condition $p > \max(d/2, 2)$ ensures that $2p' < 2^*$. Thus we have

$$\|V(x) + (w * |u_0|^2)(x)\varphi\|_{L^2} \le \frac{1}{2}\|\Delta\varphi\|_{L^2} + C\|\varphi\|_{L^2}, \quad \forall \varphi \in H^2(\mathbb{R}^d).$$

By the Kato-Rellich theorem,

$$A := -\Delta + V(x) + (w * |u_0|^2)(x) - \mu.$$

is a self-adjoint operator on $L^2(\mathbb{R}^d)$ with domain $H^2(\mathbb{R}^d)$

On the other hand, the Hartree equation can be rewritten as

$$\langle u_0, A\varphi\rangle = 0, \quad \forall \varphi \in C_c^\infty(\mathbb{R}^d).$$

Using

$$\overline{C_c^\infty(\mathbb{R}^d)}^{\|.\|_{D(A)}} = \overline{C_c^\infty(\mathbb{R}^d)}^{\|.\|_{H^2(\mathbb{R}^d)}} = H^2(\mathbb{R}^d)$$

(as $\|.\|_{D(A)}$ is comparable to $\|.\|_{H^2(\mathbb{R}^d)}$) we find that

$$\langle u_0, A\varphi\rangle = 0, \quad \forall \varphi \in H^2(\mathbb{R}^d).$$

This implies that $u_0 \in D(A^*)$. Since A is self-adjoint, we find that $u_0 \in D(A) = H^2(\mathbb{R}^d)$.

General potential. Now we consider the general case when $V = V_1 + V_2$. Define

$$A_0 := -\Delta + V_2.$$

Then A_0 is a self-adjoint operator on $L^2(\mathbb{R}^d)$ with domain

$$D(A_0) = H^2(\mathbb{R}^d) \cap D(V_2), \quad D(V_2) := \Big\{ u \in L^2(\mathbb{R}^d) \,|\, V_2 u \in L^2(\mathbb{R}^d) \Big\}$$

(exercise). Now we prove that

$$C^{-1}\Big(\|\varphi\|_{H^2} + \|V_2\varphi\|_{L^2} \Big) \le \|\varphi\|_{D(A_0)} \le \|\varphi\|_{H^2} + \|V_2\varphi\|_{L^2}, \quad \forall \varphi \in D(A_0),$$

namely the norm $\|\varphi\|_{D(A_0)}$ is equivalent to $\|\varphi\|_{H^2} + \|V_2\varphi\|_{L^2}$. Recall that $\|\varphi\|_{D(A_0)} := \|A_0\varphi\|_{L^2} + \|\varphi\|_{L^2}$. The second bound follows from the triangle inequality. For the first bound, using the IMS formula we can write

$$\begin{aligned} A_0^2 &= (-\Delta)^2 + V_2^2 + V_2(-\Delta) + (-\Delta)V_2 \\ &= (-\Delta)^2 + V_2^2 - 2(-\Delta) + (V_2+1)(-\Delta) + (-\Delta)(V_2+1) \\ &= (-\Delta)^2 + V_2^2 - 2(-\Delta) + 2\sqrt{V_2+1}(-\Delta)\sqrt{V_2+1} - 2|\nabla\sqrt{V_2+1}|^2 \\ &= (-\Delta)^2 + V_2^2 - 2(-\Delta) + 2\sqrt{V_2+1}(-\Delta)\sqrt{V_2+1} - \frac{|\nabla V_2|^2}{2(V_2+1)}. \end{aligned}$$

Then by the condition $|\nabla V_2(x)| \le C(V_2(x)+1)$ and the Cauchy-Schwarz inequality

$$\begin{aligned} A_0^2 &\ge (-\Delta)^2 + V_2^2 - 2(-\Delta) - C(V_2+1) \\ &\ge (1-\varepsilon)\Big((-\Delta)^2 + V_2^2\Big) - C_\varepsilon, \quad \forall \varepsilon \in (0,1). \end{aligned}$$

Putting differently,

$$\|A_0\varphi\|_{L^2}^2 \ge (1-\varepsilon)\|\Delta\varphi\|_{L^2(\mathbb{R}^d)}^2 + \|V\varphi\|_{L^2(\mathbb{R}^d)}^2 - C_\varepsilon\|\varphi\|_{L^2}^2, \quad \forall \varepsilon \in (0,1), \quad \forall \varphi \in D(A).$$

Thus

$$\frac{1}{C}\Big(\|\varphi\|_{H^2} + \|V_2\varphi\|_{L^2} \Big)\|\varphi\|_{D(A_0)} \le \|\varphi\|_{H^2} + \|V_2\varphi\|_{L^2}.$$

In particular, we have

$$\overline{C_c^\infty(\mathbb{R}^d)}^{D(A_0)} = D(A_0).$$

Next, using the bound

$$\|V_1(x) + (w * |u_0|^2)(x)\varphi\|_{L^2} \le \varepsilon\|\Delta\varphi\|_{L^2} + C_\varepsilon\|\varphi\|_{L^2}, \quad \forall \varphi \in H^2(\mathbb{R}^d), \quad \forall \varepsilon > 0$$

we conclude, by the Kato-Rellich theorem that

$$A := -\Delta + V(x) + (w * |u_0|^2)(x) - \mu.$$

is a self-adjoint operator on $L^2(\mathbb{R}^d)$ with domain $D(A) = D(A_0)$. The Hartree equation can be rewritten as

$$\langle u_0, A\varphi \rangle = 0, \quad \forall \varphi \in C_c^\infty(\mathbb{R}^d).$$

Using

$$\overline{C_c^\infty(\mathbb{R}^d)}^{D(A)} = \overline{C_c^\infty(\mathbb{R}^d)}^{D(A_0)} = D(A_0) = D(A).$$

we find that

$$\langle u_0, A\varphi \rangle = 0, \quad \forall \varphi \in D(A).$$

Since A is self-adjoint, we conclude that $u_0 \in D(A^*) = D(A) = H^2(\mathbb{R}^d) \cap D(V_2)$. Thus

$$-\Delta u, Vu, (w * |u_0|^2)u_0 \in L^2(\mathbb{R}^d)$$

and hence the Hartree equation holds in the usual sense of $L^2(\mathbb{R}^d)$, which is equivalent to the pointwise equality (almost everywhere). *q.e.d.*

Exercise. *Let $V : \mathbb{R}^d \to \mathbb{R}$ be a measurable function. Consider the Schrödinger operator $A = -\Delta + V(x)$ on $L^2(\mathbb{R}^d)$ with $D(A) = H^2(\mathbb{R}^d) \cap D(V)$. Prove that A is a self-adjoint operator.*

3.6 Positivity of minimizers

Theorem (Positivity of Hartree minimizers)**.** *Consider the Hartree functional*

$$\mathcal{E}_{\mathrm{H}}^V(u) := \int_{\mathbb{R}^d} \Big(|\nabla u(x)|^2 + V(x)|u(x)|^2 \Big) \mathrm{d}x + \frac{1}{2} \iint_{\mathbb{R}^d \times \mathbb{R}^d} |u(x)|^2 |u(y)|^2 w(x-y) \mathrm{d}x\mathrm{d}y$$

with $V_+ \in L^\infty_{\mathrm{loc}}(\mathbb{R}^d)$, $V_-, w \in L^p(\mathbb{R}^d) + L^\infty(\mathbb{R}^d)$, $p > \max(d/2, 1)$. Assume that the minimization problem

$$e_{\mathrm{H}}^V(\lambda) := \inf \Big\{ \mathcal{E}_{\mathrm{H}}^V(u) : u \in H^1(\mathbb{R}^d), \|u\|^2_{L^2(\mathbb{R}^d)} = \lambda \Big\}$$

has a minimizer $u_0 \in H^2(\mathbb{R}^d)$ *and it satisfies the Hartree equation*

$$\Big(-\Delta + V(x) + (w * |u_0|^2)(x) - \mu \Big) u_0(x) = 0, \quad \text{for a.e. } x \in \mathbb{R}^d.$$

Then we have

- **Positivity of minimizer:** *There exists a constant* $z \in \mathbb{C}$, $|z| = 1$ *such that*

$$z u_0(x) = |u_0(x)| > 0, \quad \text{for a.e. } x \in \mathbb{R}^d.$$

  Moreover, $|u_0|$ *is also a Hartree minimizer.*

- **Positivity of mean-field operator:** *We have*

$$-\Delta + V(x) + (w * |u_0|^2)(x) - \mu \geq 0.$$

  Moreover, this operator has the ground state energy 0*, and* $|u_0| > 0$ *is its unique ground state up to a phase factor (i.e. all ground state are given by* $z'|u_0|$ *with* $z' \in \mathbb{C}$, $|z'| = 1$*).)*

We start with recalling a very useful bound.

Theorem (Diamagnetic inequality)**.** *For any* $u \in H^1(\mathbb{R}^d)$*, we have* $|u| \in H^1(\mathbb{R}^d)$ *and*

$$|\nabla |u|(x)| \leq |\nabla u(x)|, \quad \text{for a.e. } x \in \mathbb{R}^d.$$

This is equivalent to **the convexity of gradient:** *for real-valued functions* $f, g \in H^1(\mathbb{R}^d)$*,*

$$|\nabla \sqrt{f^2 + g^2}(x)|^2 \leq |\nabla f(x)|^2 + |\nabla g(x)|^2, \quad \text{for a.e. } x \in \mathbb{R}^d.$$

In the latter bound, if we have the equality

$$|\nabla \sqrt{f^2 + g^2}(x)|^2 = |\nabla f(x)|^2 + |\nabla g(x)|^2, \quad \text{for a.e. } x \in \mathbb{R}^d.$$

and $f(x) > 0$ *for a.e.* $x \in \mathbb{R}^d$ *or* $g(x) > 0$ *for a.e.* $x \in \mathbb{R}^d$*, then* $f(x) = c g(x)$ *for a constant* c *independent of* $x \in \mathbb{R}^d$*.*

Remarks:

- The **the convexity of gradient** holds true also for complex valued functions as

$$\left|\nabla\sqrt{|f(x)|^2+|g(x)|^2}\right|^2 \le |\nabla|f|(x)|^2+|\nabla|g|(x)|^2 \le |\nabla f(x)|^2+|\nabla g(x)|^2.$$

- A more general form of the diamagnetic inequality: For any given **vector field** $\mathbf{A} \in L^2_{\rm loc}(\mathbb{R}^3,\mathbb{R}^3)$ we have the pointwise estimate

$$|\nabla|u|(x)| \le |(\nabla+\mathbf{i}\mathbf{A}(x))u(x)|, \qquad \text{for a.e. } x\in\mathbb{R}^d.$$

  This explains the name **"diamagnetic inequality"**.

Proof. **Step 1.** Consider $u=f+\mathbf{i}g$ with real-valued functions $f,g\in H^1(\mathbb{R}^d)$. Then we have the pointwise formula

$$\nabla|u|(x) = \begin{cases} 0 & \text{if } u(x)=0,\\ \dfrac{f(x)\nabla f(x)+g(x)\nabla g(x)}{|u(x)|} & \text{if } u(x)\neq 0.\end{cases}$$

In fact, for any $\varepsilon>0$ we define

$$G_\varepsilon = \sqrt{|u|^2+\varepsilon^2}-\varepsilon = \sqrt{f^2+g^2+\varepsilon^2}-\varepsilon.$$

Note that

$$0\le G_\varepsilon(x) = \frac{f^2(x)+g^2(x)}{\sqrt{f^2(x)+g^2(x)+\varepsilon^2}+\varepsilon} \le \sqrt{f^2(x)+g^2(x)} \in L^2(\mathbb{R}^d)$$

and

$$\nabla G_\varepsilon(x) = \frac{f(x)\nabla f(x)+g(x)\nabla g(x)}{\sqrt{f^2(x)+g^2(x)+\varepsilon^2}}.$$

By the Cauchy-Schwarz inequality, we have the pointwise estimate

$$|\nabla G_\varepsilon(x)| \le \frac{\sqrt{f^2(x)+g^2(x)}\sqrt{|\nabla f(x)|^2+|\nabla g(x)|^2}}{\sqrt{f^2(x)+g^2(x)+\varepsilon^2}} \le \sqrt{|\nabla f(x)|^2+|\nabla g(x)|^2}\in L^2(\mathbb{R}^d).$$

Since $\{G_\varepsilon\}$ is bounded in $H^1(\mathbb{R}^d)$ and $G_\varepsilon(x)\to|u(x)|$ pointwise as $\varepsilon\to 0$, we obtain $G_\varepsilon \rightharpoonup |u|$

weakly in $H^1(\mathbb{R}^d)$. Moreover, since

$$\nabla G_\varepsilon \to D := \begin{cases} 0 & \text{if } u(x) = 0, \\ \dfrac{f(x)\nabla f(x) + g(x)\nabla g(x)}{|u(x)|} & \text{if } u(x) \neq 0. \end{cases}$$

strongly in L^2 (by Dominated convergence), we find that $\nabla|u| = D$.

Step 2. By the Cauchy-Schwarz inequality we have, when $u(x) = f(x) + \mathbf{i}g(x) \neq 0$,

$$\begin{aligned} |\nabla|u|(x)| &= \frac{|f(x)\nabla f(x) + g(x)\nabla g(x)|}{|u(x)|} \\ &\leq \frac{\sqrt{f^2(x) + g^2(x)}\sqrt{|\nabla f(x)|^2 + |\nabla g(x)|^2}}{|u(x)|} \\ &= \sqrt{|\nabla f(x)|^2 + |\nabla g(x)|^2} = |\nabla u(x)|. \end{aligned}$$

Step 3. In the above Cauchy-Schwarz inequality, the equality

$$|\nabla\sqrt{f^2 + g^2}(x)| = \sqrt{|\nabla f(x)|^2 + |\nabla g(x)|^2}, \qquad \text{for a.e. } x \in \mathbb{R}^d.$$

occurs if and only if

$$f(x)\nabla g(x) - g(x)\nabla f(x) = 0, \qquad \text{for a.e. } x \in \mathbb{R}^d.$$

Now assume that $g(x) > 0$ for a.e. $x \in \mathbb{R}^d$ (the case $f(x) > 0$ is similar). Then the above equality implies that

$$\nabla\Big(\frac{f(x)}{g(x)}\Big) = \frac{f(x)\nabla g(x) - g(x)\nabla f(x)}{g^2(x)} = 0, \qquad \text{for a.e. } x \in \mathbb{R}^d.$$

Thus $f/g = c$ a constant. *q.e.d.*

Exercise. *Prove that if $u_n \rightharpoonup u_0$ weakly in $H^1(\mathbb{R}^d)$, then $|u_n| \rightharpoonup |u_0|$ weakly in $H^1(\mathbb{R}^d)$.*

Now we apply the diamagnetic inequality to Hartree theory.

Proof of the positivity of Hartree minimizers. **Step 1.** By the diamagnetic inequality we have

$$\mathcal{E}_{\rm H}^V(u) - \mathcal{E}_{\rm H}(|u|) = \|\nabla u\|_{L^2}^2 - \|\nabla|u|\|_{L^2}^2 \geq 0.$$

Therefore, if u_0 is a minimizer for $e_{\rm H}^V(\lambda)$, then $|u_0|$ is also a minimizer.

Step 2. Now assume that $u_0 \ge 0$ is a minimizer for $e_{\rm H}^V(\lambda)$. We prove that $u_0(x) > 0$ for all $x \in \mathbb{R}^d$. We write the Hartree equation as

$$\big(-\Delta + W(x)\big)u_0(x) = 0$$

with

$$W(x) := V(x) + (w * |u_0|^2)(x) - \mu(\lambda)$$

The special case $V_+ \in L^\infty(\mathbb{R}^d)$. Then because $w * |u_0|^2 \in L^\infty(\mathbb{R}^d)$, we have $W_+ \in L^\infty(\mathbb{R}^d)$. Thus we can take a large number $m > 0$ and rewrite the Hartree equation as

$$(-\Delta + m^2)u_0(x) = (m^2 - W)u_0(x) \ge 0, \quad \forall x \in \mathbb{R}^d.$$

Since the operator $(-\Delta + m^2)^{-1}$ is **positivity improving**, this implies that $u_0(x) > 0$ for all $x \in \mathbb{R}^d$.

Exercise (Positivity improving property)**.** *Let $m > 0$. Prove that the Yukawa potential satisfies*

$$K(x) := \int_{\mathbb{R}^d} \frac{1}{|2\pi k|^2 + m^2} e^{2\pi \mathbf{i} k\cdot x} {\rm d}k = \int_0^\infty \frac{1}{(4\pi t)^{d/2}} \exp\Big(-\frac{|x|^2}{4t} - m^2 t\Big){\rm d}t > 0.$$

Deduce that if $0 \le g \in L^2(\mathbb{R}^d)$ and $g \not\equiv 0$, then $((-\Delta + m^2)^{-1} g)(x) > 0$ for a.e. $x \in \mathbb{R}^d$.

The general case $V_+ \in L^\infty_{\rm loc}(\mathbb{R}^d)$. We have $W_+ \in L^\infty_{\rm loc}(\mathbb{R}^d)$. Thus for any $R > 0$ there exists $m > 0$ large such that

$$(-\Delta + m^2)u_0(x) = (m^2 - W(x))u_0(x) \ge 0, \quad \forall |x| < R.$$

The strict positivity $u(x) > 0$ on $|x| < R$ then follows from the following general result (see [Lieb-Loss, Analysis, Theorem 9.10] for a proof, and even a more general version).

Theorem (Harnack's inequality)**.** *Let $m > 0$ and $0 \le f \in H^2(\mathbb{R}^d)$. Assume that*

$$(-\Delta + m^2)f(x) \ge 0, \quad \textit{for a.e. } |x| \le R.$$

Then

$$f(x) \geq c_0 \int_{|y|\leq r} f(y)\mathrm{d}y, \quad \text{for a.e. } |x| \leq r < R.$$

The constant $c_0 = c_0(m, R, r) > 0$ *is independent of* f.

Since $u_0 \geq 0$ and $u_0 \not\equiv 0$, we can choose $R > 0$ large enough such that

$$\int_{|y|\leq R/2} u_0(y)\mathrm{d}y > 0.$$

Then by Harnack's inequality, from $(-\Delta + m^2)u_0(x) \geq 0$ for $|x| \leq R$ we find that

$$u_0(x) \geq c_0 \int_{|y|\leq R/2} u_0(y)\mathrm{d}y > 0, \quad \text{for a.e. } |x| \leq R/2.$$

By sending $R \to \infty$, we obtain $u_0(x) > 0$ for a.e. $x \in \mathbb{R}^d$.

Step 3. Assume that $u_0 > 0$ is a strictly positive solution to the Schrödinger equation

$$(-\Delta + W(x))u_0(x) = 0, \quad x \in \mathbb{R}^d.$$

Then 0 is the ground state energy of $-\Delta + W(x)$ and u_0 is a ground state. This follows from the following general fact.

Theorem (Perron-Frobenius Principle)**.** *Let* $0 < f \in H^2(\mathbb{R}^d)$, $W \in L^1_{\mathrm{loc}}(\mathbb{R}^d)$ *such that*

$$-\Delta f(x) + W(x)f(x) = 0, \quad \text{for a.e. } x \in \mathbb{R}^d.$$

Then $-\Delta + W \geq 0$*, namely*

$$\int_{\mathbb{R}^d} \left(|\nabla\varphi|^2 + W|\varphi|^2\right) \geq 0, \quad \forall \varphi \in C_c^\infty(\mathbb{R}^d).$$

Proof. Since $f > 0$, we can define $g = \varphi/f$. Then substituting $\varphi = fg$ we find that

$$\int |\nabla\varphi|^2 = \int |\nabla(fg)|^2 = \int |f(\nabla g)+g(\nabla f)|^2 = \int \left[|f|^2|\nabla g|^2+|g|^2|\nabla f|^2+2\Re\overline{f(\nabla g)}\cdot g(\nabla f)\right].$$

Moreover, by integration by part

$$\int |g|^2|\partial_j f|^2 = -\int f\partial_j((\partial_j f)|g|^2) = -\int f(\partial_j^2 f)|g|^2 - \int f\partial_j f(\partial_j|g|^2)$$

and hence by summing over $j = 1, 2, ..., d$

$$\int |g|^2 |\nabla f|^2 = \int f(-\Delta f)|g|^2 - 2\int f\nabla f \Re(\overline{g}(\nabla g)).$$

In summary,

$$\int |\nabla\varphi|^2 = \int |f|^2|\nabla g|^2 + \int f(-\Delta f)|g|^2.$$

Therefore,

$$\int \left(|\nabla\varphi|^2 + W|\varphi|^2\right) = \int |f|^2|\nabla g|^2 + \int f\underbrace{(-\Delta f + Wf)}_{=0}|g|^2 = \int |f|^2|\nabla g|^2 \geq 0.$$

q.e.d.

Since $C_c^\infty(\mathbb{R}^d)$ is the core domain of $-\Delta + W$, the above quadratic form estimate ensures that $-\Delta + W \geq 0$ as an operator.

Step 4. Now let us conclude. Assume that u_0 is a Hartree minimizer. By Step 1, $|u_0| \geq 0$ is also a Hartree minimizer. By Step 2, $|u_0| > 0$ pointwise. By step 3, both u_0 and $|u_0|$ are ground states for the Schrödinger operator $-\Delta + W(x)$. Let us prove that $|u_0(x)| = zu_0(x)$ for a constant $z \in \mathbb{C}$ independent of $x \in \mathbb{R}^d$.

In fact, we can write $u_0 = f + \mathbf{i}g$ with real-valued functions f, g. Then f, g are also ground states for $-\Delta+W(x)$. By the diamagnetic inequality, $|f|$ is also ground states for $-\Delta+W(x)$. Since $|f| \geq 0$, arguing as in Step 2 we conclude that $|f| > 0$.

Next, let $h \in \{f, g\}$. Since h and $|f|$ are ground states for $-\Delta + W(x)$, the function

$$\Phi := h + \mathbf{i}|f|$$

is also a ground state for $-\Delta + W(x)$. By the diamagnetic inequality again, $|\Phi|$ is also a ground state for $-\Delta + W(x)$, and moreover we have the equality

$$\int |\nabla|\Phi||^2 = \int |\nabla\Phi|^2$$

namely

$$|\nabla\sqrt{h^2(x) + f^2(x)}| = \sqrt{|\nabla h(x)|^2 + |\nabla|f|(x)|^2}, \quad \text{for a.e. } x \in \mathbb{R}^d.$$

Since $|f| > 0$, the equality case in the diamagnetic inequality tell us that $h(x) = c_h|f(x)|$ for a constant independent of x. Thus

$$u_0(x) = f(x) + \mathbf{i}g(x) = c_f|f(x)| + \mathbf{i}c_g|f(x)| = (c_f + \mathbf{i}c_g)|f(x)|$$

with $c_f + \mathbf{i}c_g$ independent of $x \in \mathbb{R}^d$. This implies that $zu_0(x) = |u_0(x)|$ for a constant $z \in \mathbb{C}$ independent of $x \in \mathbb{R}^d$. *q.e.d.*

3.7 Uniqueness of minimizers

In general, uniqueness is a hard question, and the answer depends a lot on the potentials. In this section we will focus on a simple case where the interaction potential is of **positive-type**, making the Hartree functional **convex**.

Definition (Positive-type potential)**.** *A potential $w : \mathbb{R}^d \to \mathbb{R}$ is of positive-type if $w(x-y)$ is the kernel of a positive operator on $L^2(\mathbb{R}^d)$, namely*

$$\langle f, w * f \rangle = \iint \overline{f(x)} f(y) w(x-y) \mathrm{d}x \mathrm{d}y \geq 0.$$

This property is equivalent to $\widehat{w} \geq 0$ because

$$\langle f, w * f \rangle_{L^2} = \int_{\mathbb{R}^d} \overline{\widehat{f}(k)} \widehat{w * f}(k) \mathrm{d}k = \int_{\mathbb{R}^d} |\widehat{f}(k)|^2 \widehat{w}(k) \mathrm{d}k.$$

Theorem (Uniqueness of Hartree minimizers)**.** *Consider the Hartree functional*

$$\mathcal{E}_{\mathrm{H}}(u) := \int_{\mathbb{R}^d} \Big(|\nabla u(x)|^2 + V(x)|u(x)|^2 \Big) \mathrm{d}x + \frac{1}{2} \iint_{\mathbb{R}^d \times \mathbb{R}^d} |u(x)|^2 |u(y)|^2 w(x-y) \mathrm{d}x \mathrm{d}y$$

with $V_+ \in L^\infty_{\mathrm{loc}}(\mathbb{R}^d)$, $V_-, w \in L^p(\mathbb{R}^d) + L^\infty(\mathbb{R}^d)$ with $p > \max(d/2, 1)$. Assume further

$$\widehat{w}(k) \geq 0, \qquad \text{for a.e. } k \in \mathbb{R}^d.$$

Then the followings hold true.

- **Convexity of the functional:** $0 \leq \rho \mapsto \mathcal{E}_{\mathrm{H}}^V(\sqrt{\rho})$ *is convex, namely for* $\rho_1 \geq 0$,

$\rho_2 \ge 0$ such that $\sqrt{\rho_1}, \sqrt{\rho_2} \in H^1(\mathbb{R}^d)$ and for $t \in [0,1]$,

$$t\mathcal{E}_{\rm H}^V(\sqrt{\rho_1}) + (1-t)\mathcal{E}_{\rm H}^V(\sqrt{\rho_2}) \ge \mathcal{E}_{\rm H}^V\Big(\sqrt{t\rho_1 + (1-t)\rho_2}\Big).$$

- **Uniqueness of minimizers:** *For any $\lambda > 0$ the minimization problem*

$$e_{\rm H}^V(\lambda) := \inf\Big\{\mathcal{E}_{\rm H}^V(u) : u \in H^1(\mathbb{R}^d), \|u\|_{L^2(\mathbb{R}^d)}^2 = \lambda\Big\}$$

has at most one minimizer $u_0 > 0$. This minimizer is unique up to a phase factor (i.e. all minimizers must be given by zu_0 with $z \in \mathbb{C}$, $|z| = 1$).

Proof. **Step 1.** Let $\rho_1 \ge 0$, $\rho_2 \ge 0$ such that $\sqrt{\rho_1}, \sqrt{\rho_2} \in H^1(\mathbb{R}^d)$. For any $t \in [0,1]$ we have

$$\begin{aligned} &\frac{t}{2}\iint \rho_1(x)\rho_1(y)w(x-y){\rm d}x{\rm d}y + \frac{1-t}{2}\iint \rho_2(x)\rho_2(y)w(x-y){\rm d}x{\rm d}y \\ &\quad - \frac{1}{2}\iint \Big[t\rho_1(x) + (1-t)\rho_2(x)\Big]\Big[t\rho_1(y) + (1-t)\rho_2(y)\Big]w(x-y){\rm d}x{\rm d}y \\ &= t(1-t)\iint \Big(\rho_1(x) - \rho_2(x)\Big)\Big(\rho_1(y) - \rho_2(y)\Big)w(x-y){\rm d}x{\rm d}y \ge 0. \end{aligned}$$

In the last estimate we used the fact that w is of positive-type. Combining with the convexity of the gradient term

$$t\int |\nabla\sqrt{\rho_1}|^2 + (1-t)\int |\nabla\sqrt{\rho_2}|^2 \ge \int |\nabla\sqrt{t\rho_1 + (1-t)\rho_2}|^2$$

we find that for all $t \in [0,1]$,

$$t\mathcal{E}_{\rm H}^V(\sqrt{\rho_1}) + (1-t)\mathcal{E}_{\rm H}^V(\sqrt{\rho_2}) \ge \mathcal{E}_{\rm H}^V\Big(\sqrt{t\rho_1 + (1-t)\rho_2}\Big).$$

Step 2. Assume that $e_{\rm H}^V(\lambda)$ has minimizers u_0, v_0. By a previous theorem, we know that $zu_0(x) = |u_0(x)| > 0$ and $z'v_0(x) = |v_0(x)| > 0$ with phase factors $z, z' \in \mathbb{Z}, |z| = |z'| = 1$. Moreover, $|u_0|$ and $|v_0|$ are also minimizers for $e_{\rm H}^V(\lambda)$, thanks to the diamagnetic inequality. It remains to prove that $|u_0| = |v_0|$.

By the above convexity of the Hartree functional, we have

$$e_{\rm H}^V(\lambda) = \frac{1}{2}\mathcal{E}_{\rm H}^V(|u_0|) + \frac{1}{2}\mathcal{E}_{\rm H}^V(|v_0|) \ge \mathcal{E}_{\rm H}^V\Big(\sqrt{\frac{1}{2}|u_0|^2 + \frac{1}{2}|v_0|^2}\Big) \ge e_{\rm H}^V(\lambda).$$

Here the last estimate follows from the variational principle and the constraint

$$\int \Big(\frac{1}{2}|u_0|^2 + \frac{1}{2}|v_0|^2 \Big) = \lambda.$$

Thus we must have

$$\frac{1}{2}\mathcal{E}_{\rm H}^V(|u_0|) + \frac{1}{2}\mathcal{E}_{\rm H}^V(|v_0|) = \mathcal{E}_{\rm H}^V\Big(\sqrt{\frac{1}{2}|u_0|^2 + \frac{1}{2}|v_0|^2} \Big),$$

which in particular implies that for the gradient terms

$$\frac{1}{2}\int |\nabla |u_0||^2 + \frac{1}{2}\int |\nabla |v_0||^2 = \int \Big|\nabla \sqrt{\frac{1}{2}|u_0|^2 + \frac{1}{2}|v_0|^2}\Big|^2.$$

By the diamagnetic inequality, this means that

$$\frac{1}{2}|\nabla |u_0|(x)|^2 + \frac{1}{2}|\nabla |v_0|(x)|^2 = \Big|\nabla \sqrt{\frac{1}{2}|u_0(x)|^2 + \frac{1}{2}|v_0(x)|^2}\Big|^2, \quad \text{for a.e. } x \in \mathbb{R}^d$$

and because $|u_0| > 0$, $|v_0| > 0$ we must have $|u_0| = c|v_0|$ for a phase factor c. Since

$$\int |u_0|^2 = \int |v_0|^2 = \lambda$$

the phase factor is $c = 1$. Thus we conclude that $|u_0| = |v_0|$. This completes the proof. *q.e.d.*

Note that in the above theorem, we did not discuss the existence of minimizers. In the trapping case $V(x) \to +\infty$ as $|x| \to \infty$, the existence of minimizers is guaranteed. However, in the vanishing case $V(x) \to 0$ as $|x| \to \infty$, it may happen that the minimizers do not exist if the mass is large enough. Using the convexity property, we can also prove the existence of a critical mass λ_c, where **a minimmizer exists if and only if** $\lambda \le \lambda_c$.

Theorem (Convexity and the critical mass)**.** *Consider the Hartree functional*

$$\mathcal{E}_{\rm H}(u) := \int_{\mathbb{R}^d} \Big(|\nabla u(x)|^2 + V(x)|u(x)|^2 \Big) {\rm d}x + \frac{1}{2} \iint_{\mathbb{R}^d \times \mathbb{R}^d} |u(x)|^2 |u(y)|^2 w(x-y) {\rm d}x{\rm d}y$$

and the Hartree energy

$$e_{\rm H}^V(\lambda) := \inf \Big\{ \mathcal{E}_{\rm H}^V(u) : u \in H^1(\mathbb{R}^d), \|u\|_{L^2(\mathbb{R}^d)}^2 = \lambda \Big\}$$

with $V, w \in L^p(\mathbb{R}^d) + L^q(\mathbb{R}^d)$ *with* $\infty > p, q > \max(d/2, 1)$ *and* $\widehat{w}(k) \geq 0$. *Then the followings hold true.*

- *The mapping* $\lambda \to e_{\rm H}^V(\lambda)$ *is* **convex and decreasing**. *Consequently, there exists a critical value* $0 \leq \lambda_c \leq \infty$ *such that*

$$e_{\rm H}^V(\lambda) > e_{\rm H}^V(\lambda_c) = e_{\rm H}^V(\lambda'), \quad \forall \lambda < \lambda_c \leq \lambda'.$$

  Here we used the convention $e_{\rm H}^V(0) = 0$ *and* $e_{\rm H}^V(\infty) = \infty$.

- *The minimization problem* $e_{\rm H}^V(\lambda)$ *has a minimizer* **if and only if** $\lambda \leq \lambda_c$.

Proof. Exercise! *q.e.d.*

Let us give an example where the previous abstract theorems apply.

Theorem (Hartree minimizers for bosonic atoms)**.** *Let* $Z > 0$ *and consider the Hartree functional for atoms*

$$\mathcal{E}_{\rm H}(u) := \int_{\mathbb{R}^3} \Big(|\nabla u(x)|^2 - \frac{Z}{|x|} |u(x)|^2 \Big) {\rm d}x + \frac{1}{2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{|u(x)|^2 |u(y)|^2}{|x-y|} {\rm d}x {\rm d}y.$$

and the Hartree energy

$$E(Z, \lambda) = \inf \Big\{ \mathcal{E}_{\rm H}(u) \,|\, u \in H^1(\mathbb{R}^3), \int_{\mathbb{R}^3} |u|^2 = \lambda \Big\}.$$

Then there exists a critical mass $\lambda_c = \lambda_c(Z) \in [Z, 2Z)$ *such that* $E(Z, \lambda)$ *has a minimizer if and only if* $\lambda \leq \lambda_c$. *Moreover, the minimizer is* **strictlly positive**, **unique up to a phase**, *and* **radially symmetric**.

Proof. The Coulomb potentials satisfy all relevant conditions, in particular

$$\widehat{|.|^{-1}}(k) = 4\pi |k|^{-2} > 0, \quad k \in \mathbb{R}^3.$$

The existence of the critical mass λ_c thus follows. The lower bound $\lambda_c(Z) \geq Z$ has been proved before. The upper bound $\lambda_c < 2Z$ is an exercise (c.f. Lieb's non-existence theorem for many-body Schrödinger theory). From the above discussion, we know that when exists, the minimizer u_0 is strictly positive and unique up to a phase. Morever, since the external potential $V(x) = -Z/|x|$ is radially symmetric, the Hartree functional $u \mapsto \mathcal{E}_{\rm H}^V(u)$ is rotation-invariant. Therefore, the unique minimizer $u_0 > 0$ must be radially symmetric. *q.e.d.*

Remark: For bosonic atoms the critical mass is $\lambda_c(Z) = 1.21Z$. The linearity on Z can be seen easily by scaling (**how?**). The value 1.21 is numerical. As we will see the behavior $\lambda_c(Z) \sim 1.21Z$ also holds for the many-body Schrödinger theory in the limit $Z \to \infty$.

Exercise. *Denote* $c_\alpha := \pi^{-\alpha/2}\Gamma(\alpha/2)$ *with the Gamma function*

$$\Gamma(z) = \int_0^\infty t^{z-1}e^{-t}{\rm d}t.$$

(Note that $\Gamma(n) = (n-1)!$ *for* $n \in \mathbb{N}$.*) Prove that for all* $0 < \alpha < d$ *we have*

$$\widehat{\frac{c_\alpha}{|x|^\alpha}} = \frac{c_{d-\alpha}}{|k|^{d-\alpha}}, \quad \forall k \in \mathbb{R}^d.$$

Hint: You can write

$$\frac{c_\alpha}{|x|^\alpha} = \int_0^\infty e^{-\pi\lambda|x|^2}\lambda^{\alpha/2-1}{\rm d}\lambda$$

and use the Fourier transform of the Gaussian.

3.8 Hartree theory with Dirac-delta interaction

So far we have study the Hartree theory with regular interaction potentials. The method represented in this chapter can be adapted to treat Dirac-delta potentials, which model **short-range interactions** appear often in physical set up. In this case, the Hartree theory is often called the **Gross-Pitaaevskii theory** or **nonlinear Schrödinger theory**.

Exercise. *Consider the Hartree functional with Dirac-delta interaction*

$$\mathcal{E}_{\rm H}^V(u) := \int_{\mathbb{R}^d}\Big(|\nabla u(x)|^2 + V(x)|u(x)|^2 + \frac{a}{2}|u(x)|^4\Big){\rm d}x$$

with a constant $a > 0$ *and a function* $V : \mathbb{R}^d \to \mathbb{R}$ *satisfying*

$$V_+ \in L^p_{\rm loc}(\mathbb{R}^d), \quad V_- \in L^p(\mathbb{R}^d) + L^q(\mathbb{R}^d), \quad \infty > p, q > \max(d/2, 1).$$

For every $\lambda > 0$ define

$$e_{\mathrm{H}}^{V}(\lambda) := \inf\Big\{\mathcal{E}_{\mathrm{H}}^{V}(u) : u \in H^1(\mathbb{R}^d), \|u\|_{L^2(\mathbb{R}^d)}^2 = \lambda\Big\}.$$

1. Prove that if $V(x) \to +\infty$ as $|x| \to \infty$, then $e_{\mathrm{H}}^{V}(\lambda)$ has a minimizer for all $\lambda > 0$.

2. Prove that if $V \in L^p(\mathbb{R}^d) + L^q(\mathbb{R}^d)$ and the **strict binding inequality** *holds*

$$e_{\mathrm{H}}^{V}(\lambda) < e_{\mathrm{H}}^{V}(\lambda'), \quad \forall 0 \le \lambda' < \lambda,$$

then $e_{\mathrm{H}}^{V}(\lambda)$ has a minimizer.

3. Prove that if $e_{\mathrm{H}}^{V}(\lambda)$ has a minimizer, then it has a **unique non-negative minimizer**. *(Hint: $0 \le \rho \mapsto \mathcal{E}_{\mathrm{H}}^{V}(\sqrt{\rho})$ is* **strictly convex***).*

Chapter 4

Validity of Hartree approximation

In this chapter we will derive rigorously the Hartree theory as an effective description for many-body quantum systems.

We start from many-body quantum mechanics. Consider a system of N **identical bosons** in $\mathbb{R}^d$, described by the Hamilttonian

$$H_N = \sum_{i=1}^{N}(-\Delta_{x_i} + V(x_i)) + \lambda \sum_{1\le i<j\le N} w(x_i - x_j)$$

acting on $L^2(\mathbb{R}^d)^{\otimes_s N}$. As usual, $V, w : \mathbb{R}^d \to \mathbb{R}$ and w is even. The parameter $\lambda > 0$ is used to adjust the strength of the interaction. In this chapter, we will focus on the **mean-field regime**

$$\lambda = \frac{1}{N-1}.$$

In this case, the Hartree functional obtained by taking expectation against the product state $u^{\otimes N}$ is independent of N:

$$\frac{1}{N}\langle u^{\otimes N}, H_N u^{\otimes N}\rangle = \int_{\mathbb{R}^d}\Big(|\nabla u(x)|^2+V(x)|u(x)|^2\Big)+\frac{1}{2}\iint |u(x)|^2|u(y)|^2 w(x-y)dxdy =: \mathcal{E}_{\rm H}(u).$$

We consider the ground state energy of H_N

$$E_N := \inf_{\|\Psi\|_{L^2(\mathbb{R}^d)^{\otimes_s N}}=1} \langle \Psi, H_N \Psi\rangle$$

and the Hartree energy

$$e_{\rm H} := \inf_{\|u\|_{L^2(\mathbb{R}^d)}=1} \mathcal{E}_{\rm H}(u).$$

We will prove that under appropriate conditions on V, w, the Hartree theory describes correctly the leading order behavior of the ground state energy and the ground states of H_N when $N \to \infty$.

4.1 Reduced density matrices

Definition. *For any wave function* $\Psi_N \in L^2(\mathbb{R}^d)^{\otimes_s N}$ *and any* $0 \le k \le N$*, we introduce the* k**-body reduced density matrix** $\gamma^{(k)}_{\Psi_N}$*: this is an operator on* $L^2(\mathbb{R}^d)^{\otimes_s k}$ *with kernel*

$$\gamma^{(k)}_{\Psi_N}(z_1, ..., z_k; z'_1, ..., z'_k) = \frac{N!}{(N-k)!} \int_{\mathbb{R}^{d(N-k)}} \Psi_N(z_1, ..., z_k, x_{k+1}, ..., x_N) \times \\ \times \overline{\Psi_N(z'_1, ..., z'_k, x_{k+1}, ..., x_N)} \mathrm{d}x_{k+1} ... \mathrm{d}x_N.$$

Equivalently, we can interpret $\gamma^{(k)}_{\Psi_N}$ *as the* **partial trace** *over all but the first* k *variables*

$$\gamma^{(k)}_{\Psi_N} = \frac{N!}{(N-k)!} \mathrm{Tr}_{k+1\to N} |\Psi_N\rangle\langle\Psi_N|.$$

Note that $\gamma^{(k)}_{\Psi_N}$ *is a* **non-negative, trace class operator** *on* $L^2(\mathbb{R}^d)^{\otimes_s k}$ *and*

$$\mathrm{Tr}\, \gamma^{(k)}_{\Psi_N} = \frac{N!}{(N-k)!}.$$

For example, the **one-body density matrix** $\gamma^{(1)}_{\Psi_N}$ is the operator on the one-body space $L^2(\mathbb{R}^d)$ with kernel

$$\gamma^{(1)}_{\Psi_N}(x, y) := N \int_{\mathbb{R}^{d(N-1)}} \Psi_N(x, x_2, ..., x_N) \overline{\Psi_N(y, x_2, ..., x_N)} \mathrm{d}x_2 ... \mathrm{d}x_N.$$

Its diagonal part is called the **one-body density**

$$\rho_{\Psi_N}(x) := N \int_{\mathbb{R}^{d(N-1)}} |\Psi_N(x, x_2, ..., x_N)|^2 \mathrm{d}x_2 ... \mathrm{d}x_N.$$

The function ρ_{Ψ_N} is the probability distribution of the particle density, namely $\int_\Omega \rho_{\Psi_N}$ can be interpreted as the expected number of particles in $\Omega \subset \mathbb{R}^d$; in particular

$$\int_{\mathbb{R}^d} \rho_{\Psi_N} = \operatorname{Tr} \gamma_{\Psi_N^{(1)}} = N.$$

Exercise. *Consider a wave function $\Psi_N \in L^2(\mathbb{R}^d)^{\otimes_s N}$ and a one-body operator h on $L^2(\mathbb{R}^d)$. Prove that*

$$\left\langle \Psi_N, \sum_{i=1}^N h_i \Psi_N \right\rangle = \operatorname{Tr}(h\gamma^{(1)}_{\Psi_N}).$$

Moreover, prove that for any multiplication operator $V(x)$ on $L^2(\mathbb{R}^d)$ regular enough (e.g. $V \in C_c^\infty(\mathbb{R}^d)$) we have

$$\operatorname{Tr}(V\gamma^{(1)}_{\Psi_N}) = \int_{\mathbb{R}^d} V(x)\rho_{\Psi_N}(x)\mathrm{d}x.$$

Exercise. *Let γ be a non-negative trace class operator on $L^2(\mathbb{R}^d)$ with the spectral decomposition $\gamma = \sum_{n\geq 1} \lambda_n |u_n\rangle\langle u_n|$. We define its density as*

$$\rho_\gamma(x) = \sum_{n\geq 1} \lambda_n |u_n(x)|^2.$$

Prove that if $\gamma_n \to \gamma_0$ strongly in trace class, then $\rho_{\gamma_n} \to \rho_{\gamma_0}$ strongly in $L^1(\mathbb{R}^d)$.

Remark: In physics littérature the density of an operator is often written as $\rho_\gamma(x) = \gamma(x,x)$. Mathematically, the kernel of an operator on $L^2(\mathbb{R}^d)$ is often defined for a.e. $(x,y) \in \mathbb{R}^d \times \mathbb{R}^d$, making the discussion on the "diagonal part" $\gamma(x,x)$ a bit formal (as the set $\{(x,x) \in \mathbb{R}^d\}$ has 0 measure in $\mathbb{R}^d \times \mathbb{R}^d$). However, using the spectral decomposition $\gamma = \sum_{n\geq 1} \lambda_n |u_n\rangle\langle u_n|$ we can properly define the kernel

$$\gamma(x,y) = \sum_{n\geq 1} \lambda_n u_n(x)\overline{u_n(y)}$$

which makes sense for a.e. $x, y \in \mathbb{R}^d$, and hence the formula $\rho_\gamma(x) = \gamma(x,x)$ becomes correct. An equivalent way to define the density ρ_γ without using the spectral decomposition is to use the formula

$$\operatorname{Tr}(V\gamma) = \int_{\mathbb{R}^d} V(x)\rho_\gamma(x)\mathrm{d}x$$

for all regular multiplication operators $V(x)$ on $L^2(\mathbb{R}^d)$.

The energy expectation of

$$H_N = \sum_{i=1}^N (-\Delta_{x_i} + V(x_i)) + \lambda \sum_{1\le i<j\le N} w(x_i - x_j)$$

can be rewritten conveniently using the one- and two-body density matrices

$$\Big\langle \Psi_N, H_N \Psi_N \Big\rangle = \mathrm{Tr}((-\Delta + V)\gamma^{(1)}_{\Psi_N}) + \frac{\lambda}{2}\mathrm{Tr}(w\gamma^{(2)}_{\Psi_N}).$$

The complexity of the N-body problem lies on the fact that it is very difficult to characterize the set of all two-body density matrices for N large. The so-called the **N-representability problem** is (quantum) **NP hard**, see e.g. a paper of Liu, Christandl, and Verstraete (PRL 2007).

On the other hand, the set of one-body density matrices is well-understood.

Exercise. *Let $\gamma \ge 0$ be a non-negative, trace class operator on $L^2(\mathbb{R}^d)$ with $\mathrm{Tr}\,\gamma = N$. Then there exists a wave function $\Psi_N \in L^2(\mathbb{R}^d)^{\otimes_s N}$ such that*

$$\gamma = \gamma^{(1)}_{\Psi_N}.$$

Hint: Given the spectral decomposition $\gamma = \sum_{n\ge 1}\lambda_n |u_n\rangle\langle u_n|$ you can choose

$$\Psi_N = N^{-1/2}\sum_{n\ge 1}\lambda_n^{1/2} u_n^{\otimes N}.$$

The key idea of the **mean-field approximation** is to replace the complicated two-body density matrix $\gamma^{(2)}_{\Psi_N}$ by the tensor product of the one-body density matrix

$$\gamma^{(2)}_{\Psi_N} \approx \gamma^{(1)}_{\Psi_N} \otimes \gamma^{(1)}_{\Psi_N}.$$

For the ground state energy of the Hamiltonian H_N, we will even go down to the level of one-body density ρ_{Ψ_N} and try to prove that

$$\frac{1}{N}\langle u^{\otimes N}, H_N u^{\otimes N}\rangle \approx \mathcal{E}_{\mathrm{H}}\Big(\sqrt{\frac{\rho_{\Psi_N}}{N}}\Big),$$

which eventually leads to the validity of the Hartree theory.

4.2 Hoffmann–Ostenhof inequality

The approximation

$$\frac{1}{N}\langle u^{\otimes N}, H_N u^{\otimes N}\rangle \approx \mathcal{E}_{\rm H}\Big(\sqrt{\frac{\rho_{\Psi_N}}{N}}\Big),$$

is nontrivial even for non-interacting systems. For the external potential, we have the exact identity

$$\Big\langle \Psi_N, \sum_{i=1}^N V(x_i)\Psi_N\Big\rangle = {\rm Tr}(V\gamma^{(1)}_{\Psi_N}) = \int_{\mathbb{R}^d} V(x)\rho_{\Psi_N}(x){\rm d}x.$$

However, for the kinetic operator, in general we have

$$\Big\langle \Psi_N, \sum_{i=1}^N -\Delta_{x_i}\Psi_N\Big\rangle = {\rm Tr}(-\Delta\gamma^{(1)}_{\Psi_N}) \neq \int_{\mathbb{R}^d} |\nabla\sqrt{\rho_{\Psi_N}}|^2.$$

Nevertheless, we still have the following sharp lower bound, which will be very useful to justify the Hartree approximation.

Lemma (Hoffmann–Ostenhof inequality)**.** *For every wave function $\Psi_N \in L^2(\mathbb{R}^d)^{\otimes_s N}$ we have*

$$\Big\langle \Psi_N, \sum_{i=1}^N (-\Delta_{x_i})\Psi_N\Big\rangle \geq \langle\sqrt{\rho_{\Psi_N}}, -\Delta\sqrt{\rho_{\Psi_N}}\rangle = \int_{\mathbb{R}^d} |\nabla\sqrt{\rho_{\Psi_N}}|^2.$$

Proof. **Step 1.** Since the one-body density matrix $\gamma^{(1)}_{\Psi_N}$ is a non-negative trace class operator, we have the spectral decomposition

$$\gamma^{(1)}_{\Psi_N} = \sum_{n\geq 1} |f_n\rangle\langle f_n|$$

with an orthogonal family $\{f_n\}_{n\geq 1} \subset L^2(\mathbb{R}^d)$ (the functions f_n are not necessarily normalized). Then we have the one-body density

$$\rho_{\Psi_N}(x) = \sum_{n\geq 1} |f_n(x)|^2.$$

Thus the Hoffmann–Ostenhof inequality is equivalent to

$$\sum_{n\geq 1}\int_{\mathbb{R}^d}|\nabla f_n(x)|^2 \mathrm{d}x \geq \int_{\mathbb{R}^d}\left|\nabla\sqrt{\sum_{n\geq 1}|f_n(x)|^2}\right|^2 \mathrm{d}x.$$

Step 2. We prove the latter bound for finite sums

$$\sum_{n=1}^{m}\int_{\mathbb{R}^d}|\nabla f_n(x)|^2 \mathrm{d}x \geq \int_{\mathbb{R}^d}\left|\nabla\sqrt{\sum_{n=1}^{m}|f_n(x)|^2}\right|^2 \mathrm{d}x, \quad \forall m=1,2,...$$

We can prove that by induction in m. The case $m=1$ follows from the diamagnetic inequality $|\nabla f_1(x)| \geq |\nabla |f_1|(x)|$. For $m=2$, by the diamagnetic inequality we have

$$\int_{\mathbb{R}^d}|\nabla f_1(x)|^2 \mathrm{d}x + \int_{\mathbb{R}^d}|\nabla f_2(x)|^2 \mathrm{d}x \geq \int_{\mathbb{R}^d}\left|\nabla\sqrt{|f_1(x)|^2+|f_2(x)|^2}\right|^2 \mathrm{d}x.$$

For $m=3$, using the diamagnetic inequality twice we have

$$\begin{aligned}\int_{\mathbb{R}^d}|\nabla f_1|^2 + \int_{\mathbb{R}^d}|\nabla f_2|^2 + \int_{\mathbb{R}^d}|\nabla f_3|^2 &\geq \int_{\mathbb{R}^d}\left|\nabla\sqrt{|f_1|^2+|f_2|^2}\right|^2 + \int_{\mathbb{R}^d}|\nabla f_3|^2 \\ &\geq \int_{\mathbb{R}^d}\left|\nabla\sqrt{|f_1|^2+|f_2|^2+|f_3|^2}\right|^2.\end{aligned}$$

The same applies to other values of m.

Step 3. In principle passing from finite sums to infinite sum should be easy thanks to standard density arguments. Let us explain it here. Of course it suffices to consider the case when the left side is finite. For any $m \geq 1$, denoting

$$g_m(x) = \sqrt{\sum_{n=1}^{m}|f_n(x)|^2}.$$

Then $\{g_m\}_{m\geq 1}$ is an increasing sequence and

$$0 \leq g_m(x) \leq \sqrt{\sum_{n=1}^{\infty}|f_n(x)|^2} = \sqrt{\rho_{\Psi_N}(x)} \in L^2(\mathbb{R}^d).$$

Therefore, by Lebesgue Motonone Convergence Theorem, $g_m \to \sqrt{\rho_{\Psi_N}}$ strongly in $L^2(\mathbb{R}^d)$ as

$m \to \infty$. On the other hand, we have proved in Step 2 that

$$\int_{\mathbb{R}^d} |\nabla g_m|^2 \le \sum_{n=1}^{m} \int_{\mathbb{R}^d} |\nabla f_n(x)|^2 \mathrm{d}x \le \sum_{n=1}^{\infty} \int_{\mathbb{R}^d} |\nabla f_n(x)|^2 \mathrm{d}x < \infty.$$

Thus the sequence $\{g_m\}$ is bounded in $H^1(\mathbb{R}^d)$, and hence $g_m \rightharpoonup \sqrt{\rho_{\Psi_N}}$ weakly in $H^1(\mathbb{R}^d)$. By Fatou's lemma, we conclude that

$$\int_{\mathbb{R}^d} |\nabla \sqrt{\rho_{\Psi_N}}|^2 \le \liminf_{m\to\infty} \int_{\mathbb{R}^d} |\nabla g_m|^2 \le \sum_{n=1}^{\infty} \int_{\mathbb{R}^d} |\nabla f_n(x)|^2 \mathrm{d}x = \mathrm{Tr}(-\Delta \gamma_{\Psi_N}^{(1)}).$$

q.e.d.

Remark: In general, for any operator $h \ge 0$ on $L^2(\mathbb{R}^d)$ satisfying

$$\langle u, hu\rangle \ge \langle |u|, h|u|\rangle, \quad \forall u \in L^2(\mathbb{R}^d)$$

then we have the Hoffmann–Ostenhof inequality

$$\Big\langle \Psi_N, \sum_{i=1}^{N} h_i \Psi_N \Big\rangle = \mathrm{Tr}(h\gamma_{\Psi_N}^{(1)}) \ge \langle \sqrt{\rho_{\Psi_N}}, h\sqrt{\rho_{\Psi_N}}\rangle.$$

The condition $\langle u, hu\rangle \ge \langle |u|, h|u|\rangle$ is equivalent to each of the following statements.

1. The resolvent $(h+C)^{-1}$ is **positivity preserving**, namely it maps positive functions to positive functions

$$\Big(f(x) \ge 0 \text{ for a.e. } x \in \mathbb{R}^d\Big) \Rightarrow \Big(((h+C)^{-1}f)(x) \ge 0 \text{ for a.e. } x \in \mathbb{R}^d\Big).$$

2. The operator e^{-th} is positivity preserving for all $t > 0$.

Exercise. *Let $h > 0$ be a self-adjoint operator on $L^2(\mathbb{R}^d)$ such that*

$$\Big(f(x) \ge 0 \textit{ for a.e. } x \in \mathbb{R}^d\Big) \Rightarrow \Big((e^{-th}f)(x) \ge 0 \textit{ for a.e. } x \in \mathbb{R}^d\Big), \quad \forall t > 0.$$

Prove that for any function u belongs to the quadratic form domain of h we have

$$\langle u, hu\rangle \ge \langle |u|, h|u|\rangle.$$

Since the heat kernel $e^{t\Delta}(x;y)$ is positive, the operator $e^{t\Delta}$ is positivity preserving for all $t>0$. Thus the above exercise gives an alternative proof of the diamagnetic inequality.

4.3 Onsager's lemma

Now we consider the approximation

$$\frac{1}{N}\langle u^{\otimes N}, H_N u^{\otimes N}\rangle \approx \mathcal{E}_{\rm H}\Big(\sqrt{\frac{\rho_{\Psi_N}}{N}}\Big),$$

from the angle of the interaction terms. A simple but very useful observation is

Lemma (Onsager's lemma)**.** *If $0\le \hat{w}\in L^1(\mathbb{R}^d)$, then for all $0\le g\in L^1(\mathbb{R}^d)$ we have the pointwise estimate*

$$\sum_{1\le i<j\le N} w(x_i-x_j) \ge \sum_{j=1}^N (g*w)(x_j) - \frac{1}{2}\iint g(x)g(y)w(x-y)\mathrm{d}x\mathrm{d}y - \frac{N}{2}w(0).$$

Consequently, for any wave function $\Psi_N\in L^2(\mathbb{R}^d)^{\otimes_s N}$ we have

$$\Big\langle \Psi_N, \sum_{1\le i<j\le N} w(x_i-x_j)\Psi_N\Big\rangle \ge \frac{1}{2}\iint \rho_{\Psi_N}(x)\rho_{\Psi_N}(y)w(x-y)\mathrm{d}x\mathrm{d}y - \frac{N}{2}w(0).$$

Note that the condition $\hat{w}\in L^1(\mathbb{R}^d)$ implies that $w\in L^\infty$. Thus the error term $-\frac{N}{2}w(0)$ is of order N, which is much smaller than the main term.

Proof. **Step 1.** Since $\hat{w}\ge 0$, the potential w is of positive-type. Therefore,

$$\iint \overline{f(x)}f(y)w(x-y)\mathrm{d}x\mathrm{d}y = \langle f, w*f\rangle \ge 0$$

for any "reasonable function" f. By choosing

$$f(x)=\sum_{i=1}^N \delta_0(x-x_i) - g(x)$$

with δ_0 the Dirac-delta function and using the identity $\delta_0*\varphi=\varphi$ we obtain the pointwise bound

$$\sum_{1\le i<j\le N} w(x_i - x_j) \ge \sum_{j=1}^N (g*w)(x_j) - \frac{1}{2}\iint g(x)g(y)w(x-y)\mathrm{d}x\mathrm{d}y - \frac{N}{2}w(0).$$

Remark: An alternative proof without using the Dirac-delta function: we write

$$\begin{aligned}\sum_{1\le \ell<j\le N} w(x_\ell - x_j) + \frac{N}{2}w(0) &= \frac{1}{2}\sum_{\ell,j=1}^N w(x_\ell - x_j)\\ &= \frac{1}{2}\int \widehat{w}(k)\sum_{\ell,j=1}^N e^{2\pi i k\cdot(x_\ell - x_j)}\mathrm{d}k = \frac{1}{2}\int \widehat{w}(k)\Big|\sum_{j=1}^N e^{2\pi i k\cdot x_j}\Big|^2\mathrm{d}k.\end{aligned}$$

Since $\widehat{w}(k)\ge 0$, we can complete the square

$$\Big|\sum_{j=1}^N e^{2\pi i k\cdot x_j}\Big|^2 \ge 2\Re\widehat{g}(k)\sum_{j=1}^N e^{2\pi i k\cdot x_j} - |\widehat{g}(k)|^2$$

and find that

$$\begin{aligned}\frac{1}{2}\int \widehat{w}(k)\Big|\sum_{j=1}^N e^{2\pi i k\cdot x_j}\Big|^2\mathrm{d}k &\ge \Re\int \widehat{w}(k)\widehat{g}(k)\sum_{j=1}^N e^{2\pi i k\cdot x_j}\mathrm{d}k - \frac{1}{2}\int \widehat{w}(k)|\widehat{g}(k)|^2\mathrm{d}k\\ &= \Re\sum_{j=1}^N\int \widehat{w*g}(k)e^{2\pi k\cdot x_j}\mathrm{d}k - \frac{1}{2}\int \widehat{w}(k)|\widehat{g}(k)|^2\mathrm{d}k\\ &= \sum_{j=1}^N w*g(x_j) - \frac{1}{2}\int \widehat{w}(k)|\widehat{g}(k)|^2\mathrm{d}k.\end{aligned}$$

Step 2. Now we apply the above pointwise estimate with $g=\rho_{\Psi_N}$, and then take the expectation against Ψ_N. We obtain

$$\begin{aligned}\Big\langle \Psi_N, \sum_{1\le i<j\le N} w(x_i-x_j)\Psi_N\Big\rangle &\ge \Big\langle \Psi_N, \sum_{j=1}^N (w*\rho_{\Psi_N})(x_j)\Psi_N\Big\rangle\\ &\quad - \frac{1}{2}\iint \rho_{\Psi_N}(x)\rho_{\Psi_N}(y)w(x-y)\mathrm{d}x\mathrm{d}y - \frac{N}{2}w(0)\\ &= \int \rho_{\Psi_N}(x)(w*\rho_{\Psi_N})(x)\mathrm{d}x - \frac{1}{2}\iint \rho_{\Psi_N}(x)\rho_{\Psi_N}(y)w(x-y)\mathrm{d}x\mathrm{d}y - \frac{N}{2}w(0)\\ &= \frac{1}{2}\iint \rho_{\Psi_N}(x)\rho_{\Psi_N}(y)w(x-y)\mathrm{d}x\mathrm{d}y - \frac{N}{2}w(0).\end{aligned}$$

q.e.d.

Exercise. *Consider the periodic function*

$$w(x) := \sum_{k\in\mathbb{Z}^d} \widehat{w}(k) e^{2\pi i k\cdot x}$$

with $0 \le \widehat{w} \in \ell^1(\mathbb{Z}^d)$. *Prove that for any* $N \ge 2$ *and* $\{x\}_{n=1}^N \subset \mathbb{R}^d$ *we have*

$$\sum_{1\le i<j\le N} w(x_i - x_j) \ge \frac{N^2}{2}\int_{\mathbb{R}^d} w - \frac{N}{2} w(0).$$

4.4 Convergence to Hartree energy

Theorem (Convergence to Hartree energy)**.** *Assume that*

$$V_+ \in L^\infty_{\rm loc}(\mathbb{R}^d), \quad w, V_- \in L^p(\mathbb{R}^d) + L^q(\mathbb{R}^d), \quad \infty > p, q > \max(d/2, 1).$$

Let E_N *be the ground state energy of*

$$H_N = \sum_{i=1}^N (-\Delta_{x_i} + V(x_i)) + \frac{1}{N-1} \sum_{1\le i<j\le N} w(x_i - x_j)$$

and let $e_{\rm H}$ *be the corresponding Hartree energy. Then* E_N/N *is increasing in* N *and*

$$\lim_{N\to\infty} \frac{E_N}{N} = e_{\rm H}.$$

Proof. **Step 1.** By the variational principle, it is easy to see that $E_N/N \le e_{\rm H}$. Moreover, we can prove that E_N/N is increasing as follows. By the symmetry of the wave function $\Psi_N \in L^2(\mathbb{R}^d)^{\otimes_s N}$, we can write

$$\begin{aligned}\frac{1}{N}\Big\langle \Psi_N, H_N \Psi_N \Big\rangle &= \langle \Psi_N, (-\Delta_{x_1} + V(x_1))\Psi_N\rangle + \frac{1}{2}\langle \Psi_N, w(x_1 - x_2)\Psi_N\rangle \\ &= \frac{1}{N-1}\Big\langle \Psi_N, \Big(\sum_{i=1}^{N-1}(-\Delta_{x_i} + V(x_i)) + \frac{1}{N-2}\sum_{1\le i<j\le N-1} w(x_i - x_j)\Big)\Psi_N\Big\rangle\end{aligned}$$

$$= \frac{1}{N-1}\Big\langle \Psi_N, H_{N-1}\Psi_N \Big\rangle$$

where the operator H_{N-1} acts on the first $(N-1)$ variables. By the variational principle,

$$\frac{1}{N}\Big\langle \Psi_N, H_N\Psi_N \Big\rangle = \frac{1}{N-1}\Big\langle \Psi_N, H_{N-1}\Psi_N \Big\rangle \geq \frac{E_{N-1}}{N-1}$$

for all wave functions $\Psi_N \in L^2(\mathbb{R}^d)^{\otimes_s N}$. Therefore,

$$\frac{E_N}{N} \geq \frac{E_{N-1}}{N-1}.$$

Thus E_N/N is increasing, and hence the limit exists. It remains to prove that the limit $\lim_{N\to\infty} E_N/N$ is exactly $e_{\rm H}$.

Step 2. Now we consider the "easy case" $0 \leq \widehat{w} \in L^1(\mathbb{R}^d)$. For any wave function $\Psi_N \in L^2(\mathbb{R}^d)^{\otimes_s N}$, by the Hoffmann–Ostenhof inequality we have

$$\Big\langle \Psi_N, \sum_{i=1}^N (-\Delta_{x_i} + V(x_i))\Psi_N \Big\rangle \geq \int |\nabla \sqrt{\rho_{\Psi_N}}|^2 + \int V\rho_{\Psi_N}$$

and by Onsager's lemma we have

$$\begin{aligned}\frac{1}{N-1}\Big\langle \Psi_N, \sum_{1\leq i<j\leq N} w(x_i-x_j)\Psi_N \Big\rangle &\geq \frac{1}{N-1}\Big[\frac{1}{2}\iint \rho_{\Psi_N}(x)\rho_{\Psi_N}(y)w(x-y)\mathrm{d}x\mathrm{d}y - \frac{N}{2}w(0)\Big]\\ &\geq \frac{1}{2N}\iint \rho_{\Psi_N}(x)\rho_{\Psi_N}(y)w(x-y)\mathrm{d}x\mathrm{d}y - C.\end{aligned}$$

In the last inequality we have used that w is positive-type to replace $1/(N-1)$ by $1/N$ in the main term. Thus

$$\Big\langle \Psi_N, H_N\Psi_N \Big\rangle \geq N\mathcal{E}_{\rm H}\Big(\sqrt{\frac{\rho_{\Psi_N}}{N}}\Big) - C \geq Ne_{\rm H} - C.$$

In the last estimate we have used the variational principle for $e_{\rm H}$. In conclusion we have

$$Ne_{\rm H} \geq E_N \geq Ne_{\rm H} - C$$

which implies the desired convergence $E_N/N \to e_{\rm H}$.

Step 3. Now we consider the case $\widehat{w} \in L^1(\mathbb{R}^d)$. Since $\widehat{w}$ has no sign, we will use Onsager's lemma for its positive and negative parts separately. The proof below is due to M. Lewin, using ideas of Lévy-Leblond and Lieb–Yau. We decompose

$$w = w_1 - w_2, \quad \widehat{w}_1 = (\widehat{w})_+ \geq 0, \quad \widehat{w}_2 = (\widehat{w})_- \geq 0.$$

It is more convenient to consider E_{2N}. Take a wave function $\Psi_{2N} \in L^2(\mathbb{R}^d)^{\otimes_s 2N}$. Then using the bosonic symmetry we can rewrite the expectation $\langle \Psi_{2N}, H_{2N}\Psi_{2N}\rangle$ as follows. For the one-body terms, we have

$$\begin{aligned}\Big\langle \Psi_{2N}, \sum_{i=1}^{2N}(-\Delta_{x_i} + V(x_i))\Psi_{2N}\Big\rangle &= 2N\Big\langle \Psi_{2N}, (-\Delta_{x_1} + V(x_1))\Psi_{2N}\Big\rangle \\ &= 2\Big\langle \Psi_{2N}, \sum_{i=1}^{N}(-\Delta_{x_i} + V(x_i))\Psi_{2N}\Big\rangle.\end{aligned}$$

For the interaction terms involving w_1, we write

$$\begin{aligned}\frac{1}{2N-1}\Big\langle \Psi_{2N}, \sum_{1\leq i<j\leq 2N} w_1(x_i - x_j)\Psi_{2N}\Big\rangle &= N\Big\langle \Psi_{2N}, w_1(x_1 - x_2)\Psi_{2N}\Big\rangle \\ &= \frac{2}{N-1}\Big\langle \Psi_{2N}, \sum_{1\leq i<j\leq N} w_1(x_i - x_j)\Psi_{2N}\Big\rangle.\end{aligned}$$

For the interaction terms involving w_2, we decompose as the difference of two quantities

$$\begin{aligned}&-\frac{1}{2N-1}\Big\langle \Psi_{2N}, \sum_{1\leq i<j\leq 2N} w_2(x_i - x_j)\Psi_{2N}\Big\rangle = -N\Big\langle \Psi_{2N}, w_2(x_1 - x_2)\Psi_{2N}\Big\rangle \\ &= N\Big\langle \Psi_{2N}, w_2(x_1 - x_2)\Psi_{2N}\Big\rangle - 2N\Big\langle \Psi_{2N}, w_2(x_1 - x_2)\Psi_{2N}\Big\rangle \\ &= \frac{2}{N-1}\Big\langle \Psi_{2N}, \sum_{N+1\leq i<j\leq 2N} w_2(x_i - x_j)\Psi_{2N}\Big\rangle - \frac{2}{N}\Big\langle \Psi_{2N}, \sum_{i=1}^{N}\sum_{j=N+1}^{2N} w_2(x_i - x_j)\Psi_{2N}\Big\rangle\end{aligned}$$

Thus in summary, by introducing the notations $y_k = x_{N+k}$, we can write

$$\langle \Psi_{2N}, H_{2N}\Psi_{2N}\rangle = 2\langle \Psi_{2N}, \widetilde{H}_N\Psi_{2N}\rangle$$

where

$$\widetilde{H}_N := \sum_{i=1}^{N}(-\Delta_{x_i} + V(x_i)) + \frac{1}{N-1}\sum_{1\leq i<j\leq N} w_1(x_i - x_j)$$

$$+\frac{1}{N-1}\sum_{1\le i<j\le N} w_2(y_i-y_j)-\frac{1}{N}\sum_{i=1}^{N}\sum_{j=1}^{N} w_2(y_j-x_i).$$

Next, we show that for any given $y_1,...,y_N\in\mathbb{R}^d$, the operator $\widetilde{H}_N$ of variables $x_1,...,x_N$ satisfying

$$\widetilde{H}_N\ge Ne_{\rm H}-C.$$

Indeed, for any wave function $\Phi_N\in L^2(\mathbb{R}^d)^{\otimes_s N}$, by the Hoffmann–Ostenhof inequality and Onsager's lemma (twice) we have

$$\begin{aligned}
\Big\langle\Phi_N,\widetilde{H}_N\Phi_N\Big\rangle &= \Big\langle\Phi_N,\sum_{i=1}^{N}(-\Delta_{x_i})\Phi_N\Big\rangle+\int V\rho_{\Phi_N}+\frac{1}{N-1}\Big\langle\Phi_N,\sum_{1\le i<j\le N} w_1(x_i-x_j)\Phi_N\Big\rangle\\
&\quad+\frac{1}{N-1}\sum_{1\le i<j\le N} w_2(y_i-y_j)-\frac{1}{N}\sum_{j=1}^{N}\int\rho_{\Phi_N}(x)w_2(y_j-x)\mathrm{d}x\\
&\ge\int|\nabla\sqrt{\rho_{\Phi_N}}|^2+\int V\rho_{\Phi_N}+\frac{1}{N-1}\left[\frac12\iint\rho_{\Phi_N}(x)\rho_{\Phi_N}(y)w_1(x-y)\mathrm{d}x\mathrm{d}y-\frac{N}{2}w_1(0)\right]\\
&\quad+\frac{1}{N-1}\left[\sum_{j=1}^{N}(g*w_2)(y_j)-\frac12\iint g(x)g(y)w_2(x-y)\mathrm{d}x\mathrm{d}y-\frac{N}{2}w_2(0)\right]\\
&\quad-\frac{1}{N}\sum_{j=1}^{N}(\rho_{\Phi_N}*w_2)(y_j)
\end{aligned}$$

for any function $0\le g\in L^1(\mathbb{R}^d)$. By choosing

$$g=\frac{N-1}{N}\rho_{\Phi_N}$$

we have

$$\frac{1}{N-1}\sum_{j=1}^{N}(g*w_2)(y_j)-\frac{1}{N}\sum_{j=1}^{N}(\rho_{\Phi_N}*w_2)(y_j)=0$$

and hence

$$\begin{aligned}
\Big\langle\Phi_N,\widetilde{H}_N\Phi_N\Big\rangle &\ge\int|\nabla\sqrt{\rho_{\Phi_N}}|^2+\int V\rho_{\Phi_N}+\frac{1}{2(N-1)}\iint\rho_{\Phi_N}(x)\rho_{\Phi_N}(y)w_1(x-y)\mathrm{d}x\mathrm{d}y\\
&\quad-\frac{(N-1)}{2N^2}\iint\rho_{\Phi_N}(x)\rho_{\Phi_N}(y)w_2(x-y)\mathrm{d}x\mathrm{d}y-\frac{N}{2(N-1)}\Big(w_1(0)+w_2(0)\Big)\\
&\ge\int|\nabla\sqrt{\rho_{\Phi_N}}|^2+\int V\rho_{\Phi_N}+\frac{1}{2N}\iint\rho_{\Phi_N}(x)\rho_{\Phi_N}(y)w_1(x-y)\mathrm{d}x\mathrm{d}y
\end{aligned}$$

$$
\begin{aligned}
&- \frac{1}{2N} \iint \rho_{\Phi_N}(x)\rho_{\Phi_N}(y) w_2(x-y)\mathrm{d}x\mathrm{d}y - \frac{N}{2(N-1)}\Big(w_1(0)+w_2(0)\Big) \\
&= N\mathcal{E}_{\rm H}\Big(\sqrt{\frac{\rho_{\Phi_N}}{N}}\Big) - \frac{N}{2(N-1)}\int |\widehat{w}| \ge Ne_{\rm H} - C.
\end{aligned}
$$

Since this holds for any wave function $\Phi_N \in L^2(\mathbb{R}^d)^{\otimes_s N}$, we conclude that for any given $y_1, ..., y_N \in \mathbb{R}^d$,

$$\widetilde{H}_N \ge Ne_{\rm H} - C.$$

Consequently, for any wave function $\Psi_{2N} \in L^2(\mathbb{R}^d)^{\otimes_s 2N}$ we have

$$\langle \Psi_{2N}, H_{2N}\Psi_{2N}\rangle = 2\langle \Psi_{2N}, \widetilde{H}_N \Psi_{2N}\rangle \ge 2Ne_{\rm H} - C.$$

Therefore,

$$E_{2N} \ge 2Ne_{\rm H} - C,$$

and hence

$$e_{\rm H} \ge \frac{E_{2N}}{2N} \ge e_{\rm H} - \frac{C}{N} \quad \forall N \ge 1.$$

Since $N \mapsto E_N/N$ is increasing, we conclude that

$$e_{\rm H} \ge \frac{E_N}{N} \ge e_{\rm H} - \frac{C}{N} \quad \forall N \ge 1.$$

This concludes the proof of $\lim_{N\to\infty} E_N/N = e_{\rm H}$ when $\widehat{w} \in L^1(\mathbb{R}^d)$.

Step 4. Now we consider the general case $w \in L^p(\mathbb{R}^d) + L^q(\mathbb{R}^d)$ with $\infty > p, q > \max(d/2, 1)$. Then we can take $w_\varepsilon \in C_c^\infty(\mathbb{R}^d)$ such that $w_\varepsilon \to w$ in $L^p + L^q$ as $\varepsilon \to 0^+$. More precisely, we write

$$w = f + g, \quad f \in L^p(\mathbb{R}^d), \quad g \in L^q(\mathbb{R}^d)$$

and choose

$$w_\varepsilon = f_\varepsilon + g_\varepsilon, \quad f_\varepsilon, g_\varepsilon \in C_c^\infty(\mathbb{R}^d), \quad \|f_\varepsilon - f\|_{L^p} + \|g_\varepsilon - g\|_{L^q} \le \varepsilon.$$

We take a wave function $\Psi_N \in L^2(\mathbb{R}^{dN})$ such that$\langle \Psi_N, H_N \Psi_N\rangle \le CN$. Then using

$$H_N \ge \frac{1}{2}\sum_{i=1}^N (-\Delta_{x_i}) - CN$$

(**why?**) we have the a-priori estimate

$$\Big\langle \Psi_N, \sum_{i=1}^N (-\Delta_{x_i})\Psi_N \Big\rangle \le CN.$$

By Holder's and Sobolev's inequalities, we can bound

$$\begin{aligned}
&\langle \Psi_N, |(f_\varepsilon - f)(x_1-x_2)|\Psi_N\rangle = \int_{\mathbb{R}^{dN}} |(f_\varepsilon - f)(x_1-x_2)||\Psi_N(x_1,...,x_N)|^2 \mathrm{d}x_1...\mathrm{d}x_N \\
&\le \int_{\mathbb{R}^{d(N-1)}} \Big(\int_{\mathbb{R}^d} |(f_\varepsilon - f)(x_1-x_2)|^p \mathrm{d}x_1\Big)^{1/p} \Big(\int_{\mathbb{R}^d} |\Psi_N(x_1,...,x_N)|^{2p'}\mathrm{d}x_1\Big)^{1/p'} \mathrm{d}x_2...\mathrm{d}x_N \\
&\le C\|f_\varepsilon - f\|_{L^p(\mathbb{R}^d)} \langle \Psi_N, (1-\Delta_{x_1})\Psi_N\rangle.
\end{aligned}$$

Here $\frac{1}{p}+\frac{1}{p'}=1$ and the condition $p>\max(d/2,1)$ implies that $2p' \in (2,2^*)$. Similarly,

$$\langle \Psi_N, |(g_\varepsilon - g)(x_1-x_2)|\Psi_N\rangle \le C\|g_\varepsilon - g\|_{L^q(\mathbb{R}^d)} \langle \Psi_N, (1-\Delta_{x_1})\Psi_N\rangle.$$

Using the choice of $f_\varepsilon, g_\varepsilon$ and the bosonic symmetry we deduce that

$$\frac{1}{N-1}\sum_{1\le i<j\le N} \langle \Psi_N, (w-w_\varepsilon)(x_i-x_j)\Psi_N\rangle \ge -C\varepsilon \sum_{i=1}^N \langle \Psi_N, (1-\Delta_{x_i})\Psi_N\rangle \ge -C\varepsilon N.$$

On the other hand, since $w_\varepsilon \in C_c^\infty(\mathbb{R}^d)$, we have $\widehat{w}_\varepsilon \in L^1(\mathbb{R}^d)$ and from Step 3 we get

$$\sum_{i=1}^N (-\Delta_{x_i} + V(x_i)) + \frac{1}{N-1}\sum_{1\le i<j\le N} w_\varepsilon(x_i-x_j) \ge N e_{\mathrm{H},\varepsilon} - C_\varepsilon$$

where

$$e_{\mathrm{H},\varepsilon} := \inf_{\|u\|_{L^2(\mathbb{R}^d)}=1} \Big\{ \int (|\nabla u|^2 + V|u|^2) + \frac{1}{2}\iint |u(x)|^2|u(y)|^2 w_\varepsilon(x-y)\mathrm{d}x\mathrm{d}y \Big\}.$$

Thus in summary, we obtain the lower bound

$$\langle \Psi_N, H_N\Psi_N\rangle \ge N e_{\mathrm{H},\varepsilon} - C_\varepsilon - C\varepsilon N$$

for any wave function Ψ_N satisfying $\langle \Psi_N, H_N\Psi_N\rangle \le CN$. This implies that

$$\lim_{N\to\infty} \frac{E_N}{N} \ge e_{\mathrm{H},\varepsilon} - C\varepsilon, \quad \forall \varepsilon > 0.$$

The conclusion follows from the fact that $e_{\mathrm{H},\varepsilon} \to e_{\mathrm{H}}$ as $\varepsilon \to 0$ (exercise). *q.e.d.*

Exercise. *Assume that*

$$V_+ \in L^\infty_{\mathrm{loc}}(\mathbb{R}^d), \quad w_0, V_- \in L^p(\mathbb{R}^d) + L^q(\mathbb{R}^d), \quad \infty > p, q > \max(d/2, 1).$$

Let $w_\varepsilon \to w_0$ *in* $L^p + L^q$ *as* $\varepsilon \to 0^+$ *and define the Hartree energy*

$$e_{\mathrm{H},\varepsilon} := \inf_{\|u\|_{L^2(\mathbb{R}^d)}=1} \Big\{ \int_{\mathbb{R}^d} (|\nabla u|^2 + V|u|^2) + \frac{1}{2} \iint_{\mathbb{R}^d \times \mathbb{R}^d} |u(x)|^2 |u(y)|^2 w_\varepsilon(x-y) \mathrm{d}x \mathrm{d}y \Big\}.$$

Prove that $e_{\mathrm{H},\varepsilon} \to e_{\mathrm{H},0}$ *as* $\varepsilon \to 0^+$.

4.5 Convergence to Hartree minimizer

Now we turn to the convergence of ground states. Heuristically, if Ψ_N is a ground state of H_N, or more generally an **approximate ground state**, i.e.

$$\langle \Psi_N, H_N \Psi_N \rangle = E_N + o(N)_{N\to\infty},$$

then we expect that

$$\Psi_N \approx u_0^{\otimes N}$$

where u_0 is a Hartree minimizer. Here the approximation $\Psi_N \approx u_0^{\otimes N}$ means that most of the particles in the N-body state Ψ_N occupy a common one-body state u_0. This phenomenon is called **the Bose-Einstein condensation** (BEC). Note that the approximation $\Psi_N \approx u_0^{\otimes N}$ has to be understood in an appropriate sense. In fact, Ψ_N and $u_0^{\otimes N}$ are **not close in the usual norm** of the Hilbert space $L^2(\mathbb{R}^d)^{\otimes_s N}$ (except the non-interacting case). The proper meaning of the Bose-Einstein condensation can be formulated in terms of reduced density matrices.

Definition. *Consider the quantum states* $\{\Psi_N\}_{N\geq 1}$, *where* Ψ_N *is a wave function in* $L^2(\mathbb{R}^d)^{\otimes_s N}$. *We say that there is* **the complete Bose-Einstein condensation** *if there* *exists a one-body state $u_0 \in L^2(\mathbb{R}^d)$ such that*

$$\lim_{N\to\infty} \frac{\langle u_0, \gamma^{(1)}_{\Psi_N} u_0\rangle}{N} = 1.$$

Remarks:

- If $\Psi_N = u_0^{\otimes N}$, then $\gamma^{(1)}_{\Psi_N} = N|u_0\rangle\langle u_0|$, and hence

$$\frac{\langle u_0, \gamma^{(1)}_{\Psi_N} u_0\rangle}{N} = 1.$$

- For any wave function $\Psi_N \in L^2(\mathbb{R}^d)^{\otimes_s N}$, $\langle u_0, \gamma^{(1)}_{\Psi_N} u_0\rangle$ is interpreted as the expectation of the particle number in the condensate state u_0. In general, we always have

$$\langle u_0, \gamma^{(1)}_{\Psi_N} u_0\rangle \le \mathrm{Tr}(\gamma^{(1)}_{\Psi_N}) = N.$$

  The complete BEC means that we have the lower bound

$$\langle u_0, \gamma^{(1)}_{\Psi_N} u_0\rangle \ge N + o(N).$$

- By the variational principle, the complete BEC is equivalent to the fact that **the largest eigenvalue of $\gamma^{(1)}_{\Psi_N}$ is** $N + o(N)$. Further equivalent statements of the BEC are in the following exercise.

Exercise. *Consider the quantum states $\{\Psi_N\}_{N\ge 1}$, where Ψ_N is a wave function in $L^2(\mathbb{R}^d)^{\otimes_s N}$. Let $u_0 \in L^2(\mathbb{R}^d)$. Prove that the following statements are equivalent.*

1. $\lim_{N\to\infty} N^{-1}\langle u_0, \gamma^{(1)}_{\Psi_N} u_0\rangle = 1$.
2. $N^{-1}\gamma^{(1)}_{\Psi_N} \to |u_0\rangle\langle u_0|$ *strongly in the operator norm.*
3. $N^{-1}\gamma^{(1)}_{\Psi_N} \to |u_0\rangle\langle u_0|$ *strongly in the trace class norm.*

Hint: $A = N^{-1}\gamma^{(1)}_{\Psi_N} - |u_0\rangle\langle u_0|$ has trace 0, and exactly one negative eigenvalue (except if $A = 0$).

In principle, the BEC is not equivalent to convergence of ground states. In fact, proving the BEC is often more difficult than proving the convergence of ground states.

Theorem (Convergence to Hartree minimizer: "easy case")**.** *Assume that*

- $0 \le \widehat{w} \in L^1(\mathbb{R}^d)$;
- $V \in L^\infty_{\rm loc}(\mathbb{R}^d)$ *and* $V(x) \to +\infty$ *as* $|x| \to \infty$.

Let $\Psi_N \in L^2(\mathbb{R}^d)^{\otimes_s N}$ *be an* **approximate ground state** *of*

$$H_N = \sum_{i=1}^N (-\Delta_{x_i} + V(x_i)) + \frac{1}{N-1} \sum_{1 \le i < j \le N} w(x_i - x_j).$$

Then we have the **complete BEC with optimal error estimate**

$$\langle u_0, \gamma^{(1)}_{\Psi_N} u_0 \rangle = N + \mathcal{O}(1).$$

Here u_0 *is the unique Hartree minimizer (up to a phase factor).*

Proof. **Step 1.** Similarly to the previous section, using $0 \le \widehat{w} \in L^1(\mathbb{R}^d)$ and Onsager's lemma we have

$$\begin{aligned}\frac{1}{N-1}\Big\langle \Psi_N, \sum_{1\le i<j\le N} w(x_i - x_j)\Psi_N \Big\rangle &\ge \frac{1}{N-1}\Big[\frac{1}{2}\iint \rho_{\Psi_N}(x)\rho_{\Psi_N}(y) w(x-y) {\rm d}x{\rm d}y - \frac{N}{2}w(0)\Big] \\ &\ge \frac{1}{2N}\iint \rho_{\Psi_N}(x)\rho_{\Psi_N}(y) w(x-y) {\rm d}x{\rm d}y - C.\end{aligned}$$

For the kinetic term, we do not use the Hoffmann–Ostenhof inequality. Thus we get

$$\Big\langle \Psi_N, H_N \Psi_N \Big\rangle \ge {\rm Tr}((-\Delta + V)\gamma^{(1)}_{\Psi_N}) + \frac{1}{2N}\iint \rho_{\Psi_N}(x)\rho_{\Psi_N}(y) w(x-y) {\rm d}x{\rm d}y - C.$$

Here we keep the one-body density matrix because it is the relevant object for the BEC.

Step 2. The new idea now is to linearize the non-linear term. Since w is of positive-type, we can use

$$\iint \overline{f(x)} f(y) w(x-y) {\rm d}x{\rm d}y \ge 0$$

with $f = \rho_{\Psi_N}(x) - N|u_0|^2$ with u_0 the Hartree minimizer. This gives

$$\begin{aligned}&\frac{1}{2N}\iint \rho_{\Psi_N}(x)\rho_{\Psi_N}(y) w(x-y) {\rm d}x{\rm d}y \\ &\ge \iint \rho_{\Psi_N}(x)|u_0(y)|^2 w(x-y) {\rm d}x{\rm d}y - \frac{N}{2}\iint |u_0(x)|^2|u_0(y)|^2 w(x-y) {\rm d}x{\rm d}y.\end{aligned}$$

Recall that under our conditions on w, V, the existence and uniqueness of the Hartree minimizer u_0 have been proved in the previous chapter. Moreover, we have the Hartree equation

$$h_{\rm mf} u_0 = 0, \quad h_{\rm mf} := -\Delta + V + (w * |u_0|^2) - \mu$$

with the chemical potential

$$\begin{aligned}\mu &= \int_{\mathbb{R}^d} \Big(|\nabla u_0(x)|^2 + V(x)|u_0(x)|^2 \Big) {\rm d}x + \iint_{\mathbb{R}^d \times \mathbb{R}^d} |u_0(x)|^2 |u_0(y)|^2 w(x-y) {\rm d}x {\rm d}y \\ &= e_{\rm H} + \frac{1}{2} \iint_{\mathbb{R}^d \times \mathbb{R}^d} |u_0(x)|^2 |u_0(y)|^2 w(x-y) {\rm d}x {\rm d}y.\end{aligned}$$

Thus

$$\begin{aligned}&\frac{1}{2N} \iint \rho_{\Psi_N}(x) \rho_{\Psi_N}(y) w(x-y) {\rm d}x {\rm d}y \\ &\ge \iint \rho_{\Psi_N}(x) |u_0(y)|^2 w(x-y) {\rm d}x {\rm d}y - \frac{N}{2} \iint |u_0(x)|^2 |u_0(y)|^2 w(x-y) {\rm d}x {\rm d}y \\ &= \int \rho_{\Psi_N} (|u_0|^2 * w) + N(e_{\rm H} - \mu) = N e_{\rm H} + {\rm Tr} \Big((|u_0|^2 * w - \mu) \gamma^{(1)}_{\Psi_N} \Big).\end{aligned}$$

Combining the latter bound with the previous bound on $\Big\langle \Psi_N, H_N \Psi_N \Big\rangle$ we deduce that

$$\begin{aligned}\Big\langle \Psi_N, H_N \Psi_N \Big\rangle &\ge {\rm Tr} \Big((-\Delta + V) \gamma^{(1)}_{\Psi_N} \Big) + \frac{1}{2N} \iint \rho_{\Psi_N}(x) \rho_{\Psi_N}(y) w(x-y) {\rm d}x {\rm d}y - C \\ &\ge N e_{\rm H} + {\rm Tr} \Big(h_{\rm mf} \gamma^{(1)}_{\Psi_N} \Big) - C.\end{aligned}$$

Thanks to the uniform upper bound $\Big\langle \Psi_N, H_N \Psi_N \Big\rangle \le N e_{\rm H}$, we conclude that

$${\rm Tr} \Big(h_{\rm mf} \gamma^{(1)}_{\Psi_N} \Big) \le C.$$

Step 3. From the Hartree theory, we know that the one-body Schrödinger operator

$$h_{\rm mf} := -\Delta + V + (w * |u_0|^2) - \mu$$

has the lowest eigenvalue 0 and u_0 is its unique ground state (up to a phase factor). Moreover, since $V(x) \to \infty$ when $|x| \to \infty$, $h_{\rm mf}$ has compact resolvent. Thus it has eigenvalues

$$0 = \lambda_1 < \lambda_2 \le \lambda_3 \le ...$$

The strict inequality $\lambda_1 < \lambda_2$ is called the **spectral gap**. By the min-max principle, if we introduce the projection

$$P = |u_0\rangle\langle u_0|, \quad Q = 1 - P,$$

then we have $h_{\rm mf} P = P h_{\rm mf} = 0$ and

$$h_{\rm mf} Q = Q h_{\rm mf} Q \geq (\lambda_2 - \lambda_1) Q.$$

Next, let us decompose

$$\gamma^{(1)}_{\Psi_N} = (P+Q)\gamma^{(1)}_{\Psi_N}(P+Q) = P\gamma^{(1)}_{\Psi_N}P + P\gamma^{(1)}_{\Psi_N}Q + Q\gamma^{(1)}_{\Psi_N}P + Q\gamma^{(1)}_{\Psi_N}Q.$$

Then by the above properties of $h_{\rm mf}P, h_{\rm mf}Q$ and the cyclicity of the trace we have

$$\operatorname{Tr}\left(h_{\rm mf}\gamma^{(1)}_{\Psi_N}\right) = \operatorname{Tr}\left(h_{\rm mf}Q\gamma^{(1)}_{\Psi_N}Q\right) = \operatorname{Tr}\left(Qh_{\rm mf}Q\gamma^{(1)}_{\Psi_N}\right) \geq (\lambda_2 - \lambda_1)\operatorname{Tr}\left(Q\gamma^{(1)}_{\Psi_N}\right).$$

Combining with the previous bound

$$\operatorname{Tr}\left(h_{\rm mf}\gamma^{(1)}_{\Psi_N}\right) \leq C.$$

and the spectral gap $\lambda_2 - \lambda_1 > 0$ we conclude that

$$C \geq \operatorname{Tr}\left(Q\gamma^{(1)}_{\Psi_N}\right) = \operatorname{Tr}\left((1-P)\gamma^{(1)}_{\Psi_N}\right) = N - \langle u_0, \gamma^{(1)}_{\Psi_N} u_0\rangle.$$

This completes the proof of the BEC. *q.e.d.*

Theorem (Convergence to Hartree minimizer: general case)**.** *Assume that*

- $V_+ \in L^\infty_{\rm loc}(\mathbb{R}^d), \quad w, V_- \in L^p(\mathbb{R}^d) + L^q(\mathbb{R}^d), \quad \infty > p, q > \max(d/2, 1).$
- *The Hartree problem* $e_{\rm H} = \inf_{\|u\|_{L^2}=1} \mathcal{E}_{\rm H}(u)$ *has a* **unique minimizer** u_0 *(up to a phase factor). Moreover, any minimizing sequence of* $e_{\rm H}$ *has a subsequence converging to* u_0 *(up to a phase) strongly in* $L^2(\mathbb{R}^d)$*.*

Let $\Psi_N \in L^2(\mathbb{R}^d)^{\otimes_s N}$ *be an approximate ground state for*

$$H_N = \sum_{i=1}^N (-\Delta_{x_i} + V(x_i)) + \frac{1}{N-1}\sum_{1\leq i<j\leq N} w(x_i - x_j).$$

Then we have the **complete Bose-Einstein condensation**

$$\lim_{N\to\infty} \frac{\langle u_0, \gamma^{(1)}_{\Psi_N} u_0\rangle}{N} = 1.$$

Remarks:

- For the complete BEC on u_0 to hold, u_0 must be the **unique Hartree minimizer** (up to a phase factor). In fact, if v_0 is another Hartree minimizer, then $v_0^{\otimes N}$ is an approximate ground state and $\gamma^{(1)}_{v_0^{\otimes N}} = N|v_0\rangle\langle v_0|$. Therefore,

$$1 = \lim_{N\to\infty} \frac{\langle u_0, \gamma^{(1)}_{\Psi_N} u_0\rangle}{N} = |\langle u_0, v_0\rangle|^2$$

  implies that v_0 is equal to u_0 up to a phase factor.

- The **pre-compactness** of the minimizing sequences holds when either $V(x) \to \infty$ as $|x| \to \infty$, or $V \in L^p(\mathbb{R}^d) + L^q(\mathbb{R}^d)$ and we have **the strict binding inequality**

$$e^V_{\rm H}(1) < e^V_{\rm H}(\lambda) + e^0_{\rm H}(1-\lambda), \quad \forall 0 \le \lambda < 1.$$

Proof. We will use the **Hellmann-Feynman argument**, a general method to derive the information on ground states from the ground state energy of perturbed Hamiltonians.

Step 1. For any $\varepsilon > 0$, we define the **perturbed N-body Hamiltonian**

$$H_{N,\varepsilon} = H_N + \varepsilon \sum_{i=1}^N P_{x_i}, \quad P = |u_0\rangle\langle u_0|$$

and call $E_{N,\varepsilon}$ the ground state energy of $H_{N,\varepsilon}$. We prove that the complete BEC follows from the following claim:

$$\liminf_{\varepsilon\to 0^+} \liminf_{N\to\infty} \frac{E_{N,\varepsilon} - E_N}{\varepsilon N} \ge 1.$$

Indeed, assume that the latter inequality holds true. Let $\Psi_N \in L^2(\mathbb{R}^d)^{\otimes_s N}$ be an approximate ground state for H_N. Then by the variational principle, we have

$$\varepsilon\langle u_0, \gamma^{(1)}_{\Psi_N} u_0\rangle = \langle \Psi_N, H_{N,\varepsilon}\Psi_N\rangle - \langle \Psi_N, H_N\Psi_N\rangle \ge E_{N,\varepsilon} - E_N + o(N),$$

and hence

$$\liminf_{N\to\infty} \frac{\langle u_0, \gamma^{(1)}_{\Psi_N} u_0\rangle}{N} \ge \liminf_{\varepsilon\to 0^+} \liminf_{N\to\infty} \frac{E_{N,\varepsilon} - E_N + o(N)}{\varepsilon N} \ge 1.$$

Step 2. Now we estimate $E_{N,\varepsilon} - E_N$. By the convergence to Hartree energy, we know that

$$E_N = Ne_{\rm H} + o(N)$$

where

$$e_{\rm H} := \inf_{\|u\|_{L^2(\mathbb{R}^d)}=1} \Big\{ \int_{\mathbb{R}^d} (|\nabla u|^2 + V|u|^2) + \frac{1}{2} \iint_{\mathbb{R}^d\times\mathbb{R}^d} |u(x)|^2|u(y)|^2 w(x-y) {\rm d}x{\rm d}y \Big\}.$$

For our purpose, it is useful to introduce the **Hartree energy for mixed states**

$$\widetilde{e}_{\rm H} := \inf_{\substack{\gamma\ge 0 \text{ on } L^2(\mathbb{R}^d)\\ \operatorname{Tr}\gamma=1}} \Big\{ \operatorname{Tr}((-\Delta+V)\gamma) + \frac{1}{2} \iint_{\mathbb{R}^d\times\mathbb{R}^d} \rho_\gamma(x)\rho_\gamma(y) w(x-y) {\rm d}x{\rm d}y \Big\}.$$

Here recall that $\rho_\gamma(x) = \gamma(x,x)$ is the density of γ (defined properly by spectral decomposition). At first sight, it does not look very useful because $e_{\rm H}$ and $\widetilde{e}_{\rm H}$ coincide!

Exercise. *Prove that $e_{\rm H} = \widetilde{e}_{\rm H}$. Hint: You can use the Hoffmann-Ostenhof inequality.*

However, the advantage of $\widetilde{e}_{\rm H}$ is that its definition can be extended easily to the perturbed problem. For any $\varepsilon > 0$, we define

$$\widetilde{e}_{{\rm H},\varepsilon} := \inf_{\substack{\gamma\ge 0 \text{ on } L^2(\mathbb{R}^d)\\ \operatorname{Tr}\gamma=1}} \Big\{ \operatorname{Tr}((-\Delta+V+\varepsilon P)\gamma) + \frac{1}{2} \iint_{\mathbb{R}^d\times\mathbb{R}^d} \rho_\gamma(x)\rho_\gamma(y) w(x-y) {\rm d}x{\rm d}y \Big\}.$$

This is the relevant limit of the perturbed N-body energy $E_{N,\varepsilon}$.

Exercise. *Prove that*

$$\lim_{N\to\infty} \frac{E_{N,\varepsilon}}{N} = \widetilde{e}_{{\rm H},\varepsilon}.$$

Hint: You can follow exactly the proof of the "Convergence to Hartree energy", without using the Hoffmann-Ostenhof inequality.

Thus we have proved that for any $\varepsilon > 0$,

$$\lim_{N\to\infty} \frac{E_{N,\varepsilon} - E_N}{N} = \widetilde{e}_{{\rm H},\varepsilon} - e_{\rm H}.$$

Step 3. Finally, we prove that

$$\lim_{\varepsilon\to 0^+} \frac{\widetilde{e}_{{\rm H},\varepsilon} - e_{\rm H}}{\varepsilon} = 1.$$

The upper bound $\widetilde{e}_{\mathrm{H},\varepsilon} \le e_{\mathrm{H}} + \varepsilon$ follows by choosing the trial state $\gamma = |u_0\rangle\langle u_0|$ for $\widetilde{e}_{\mathrm{H},\varepsilon}$. It remains to prove the lower bound.

Let γ_ε be an approximate ground state for $\widetilde{e}_{\mathrm{H},\varepsilon}$, namely $\gamma_\varepsilon \ge 0$ on $L^2(\mathbb{R}^d)$, $\mathrm{Tr}(\gamma_\varepsilon) = 1$ and

$$\widetilde{\mathcal{E}}_{\mathrm{H},\varepsilon}(\gamma_\varepsilon) := \mathrm{Tr}((-\Delta + V + \varepsilon P)\gamma_\varepsilon) + \frac{1}{2}\iint_{\mathbb{R}^d\times\mathbb{R}^d} \rho_{\gamma_\varepsilon}(x)\rho_{\gamma_\varepsilon}(y)w(x-y)\mathrm{d}x\mathrm{d}y \le \widetilde{e}_{\mathrm{H},\varepsilon} + o(\varepsilon).$$

The key point is to prove that

$$\mathrm{Tr}(P\gamma_\varepsilon) = \langle u_0, \gamma_\varepsilon u_0\rangle \to 1.$$

If the latter convergence holds, then by the Hoffmann-Ostenhof inequality we find that

$$\widetilde{\mathcal{E}}_{\mathrm{H},\varepsilon}(\gamma_\varepsilon) \ge \mathcal{E}_{\mathrm{H}}(\sqrt{\rho_{\gamma_\varepsilon}}) + \varepsilon\langle u_0, \gamma_\varepsilon u_0\rangle \ge e_{\mathrm{H}} + \varepsilon + o(\varepsilon)$$

and the lower bound $\widetilde{e}_{\mathrm{H},\varepsilon} \ge e_{\mathrm{H}} + \varepsilon + o(\varepsilon)$ follows. Thus it remains to show that $\langle u_0, \gamma_\varepsilon u_0\rangle \to 1$.

Convergence of density $\rho_{\gamma_\varepsilon}$. By the Hoffmann-Ostenhof inequality and the upper bound $\widetilde{e}_{\mathrm{H},\varepsilon} \le e_{\mathrm{H}} + \varepsilon$, we find that

$$\mathcal{E}_{\mathrm{H}}(\sqrt{\rho_{\gamma_\varepsilon}}) \le \mathcal{E}_{\mathrm{H}}(\sqrt{\rho_{\gamma_\varepsilon}}) + \varepsilon\,\mathrm{Tr}(P\gamma_\varepsilon) \le \widetilde{\mathcal{E}}_{\mathrm{H},\varepsilon}(\gamma_\varepsilon) \le \widetilde{e}_{\mathrm{H},\varepsilon} + o(\varepsilon) \le e_{\mathrm{H}} + O(\varepsilon).$$

Thus $\sqrt{\rho_{\gamma_\varepsilon}}$ is a miminizing sequence for e_{H} when $\varepsilon \to 0^+$. Thanks to the assumption on the pre-compactness of minimizing sequences for e_{H}, up to a subsequence as $\varepsilon \to 0^+$ and up to a phase factor of u_0, we have $\sqrt{\rho_{\gamma_\varepsilon}} \to u_0 \ge 0$ strongly in $L^2(\mathbb{R}^d)$. Since $\sqrt{\rho_{\gamma_\varepsilon}}$ is bounded in $H^1(\mathbb{R}^d)$ (as $\mathcal{E}_{\mathrm{H}}(\sqrt{\rho_{\gamma_\varepsilon}})$ is bounded), by Sobolev's inequality we obtain

$$\sqrt{\rho_{\gamma_\varepsilon}} \to u_0 \text{ strongly in } L^r(\mathbb{R}^d) \text{ for all } r \in [2, 2^*).$$

Linearized equation. Using $\sqrt{\rho_{\gamma_\varepsilon}} \to u_0$ in $L^r(\mathbb{R}^d)$ for all $r \in [2, 2^*)$ and the assumption $w \in L^p + L^q$, we get

$$\frac{1}{2}\iint_{\mathbb{R}^d\times\mathbb{R}^d} (\rho_{\gamma_\varepsilon}(x) - |u_0(x)|^2)(\rho_{\gamma_\varepsilon}(y) - |u_0(y)|^2)w(x-y)\mathrm{d}x\mathrm{d}y \to 0$$

which is equivalent to

$$\frac{1}{2}\iint \rho_{\gamma_\varepsilon}(x)\rho_{\gamma_\varepsilon}(y)w(x-y)\mathrm{d}x\mathrm{d}y = \iint |u_0(x)|^2\rho_{\gamma_\varepsilon}(y)w(x-y)\mathrm{d}x\mathrm{d}y$$

$$- \frac{1}{2} \iint |u_0(x)|^2 |u_0(y)|^2 w(x-y) \mathrm{d}x \mathrm{d}y + o(1)$$
$$= \int (|u_0|^2 * w) \rho_{\gamma_\varepsilon} + e_{\mathrm{H}} - \mu$$

where

$$\mu = \int_{\mathbb{R}^d} \Big(|\nabla u_0(x)|^2 + V(x)|u_0(x)|^2 \Big) \mathrm{d}x + \iint_{\mathbb{R}^d \times \mathbb{R}^d} |u_0(x)|^2 |u_0(y)|^2 w(x-y) \mathrm{d}x \mathrm{d}y$$

is the chemical potential in the Hartree equation

$$h_{\mathrm{mf}} u_0 = 0, \quad h_{\mathrm{mf}} := -\Delta + V + (w * |u_0|^2) - \mu \ge 0.$$

Thus

$$\widetilde{\mathcal{E}}_{\mathrm{H},\varepsilon}(\gamma_\varepsilon) = e_{\mathrm{H}} + \mathrm{Tr}(h_{\mathrm{mf}} \gamma_\varepsilon) + \varepsilon \langle u_0, \gamma_\varepsilon u_0 \rangle + o(1).$$

Consequently,

$$\mathrm{Tr}(h_{\mathrm{mf}} \gamma_\varepsilon) \to 0.$$

Weak-limit in Hilbert-Schmidt topology. Using the operator lower bound

$$h_{\mathrm{mf}} \ge -\frac{1}{2}\Delta - C$$

we find that

$$\mathrm{Tr}((1-\Delta)\gamma_\varepsilon) = \mathrm{Tr}((1-\Delta)^{1/2} \gamma_\varepsilon (1-\Delta)^{1/2}) \le C.$$

Thus $(1-\Delta)^{1/2}\gamma_\varepsilon(1-\Delta)^{1/2}$ is bounded in trace class, and hence it is bounded in the Hilbert-Schmidt topology. By the Banach-Alaoglu theorem for the Hilbert-Schmidt space, up to a subsequence $\varepsilon \to 0^+$ we have

$$(1-\Delta)^{1/2}\gamma_\varepsilon(1-\Delta)^{1/2} \rightharpoonup (1-\Delta)^{1/2}\gamma_0(1-\Delta)^{1/2}$$

weakly in the Hilbert-Schmidt topology, namely

$$\mathrm{Tr}(K(1-\Delta)^{1/2}\gamma_\varepsilon(1-\Delta)^{1/2}) \to \mathrm{Tr}(K(1-\Delta)^{1/2}\gamma_0(1-\Delta)^{1/2}), \quad \forall K \text{ Hilbert-Schmidt operators.}$$

for a non-negative trace class operator $\gamma_0 \ge 0$ on $L^2(\mathbb{R}^d)$ (exercise). From this weak convergence and the fact that $\rho_{\gamma_\varepsilon} \to |u_0|^2$ strongly in $L^1(\mathbb{R}^d)$, we deduce that $\rho_{\gamma_0} = |u_0|^2$ (exercise).

Let us determine the limit γ_0. Since $\gamma_\varepsilon \rightharpoonup \gamma_0$ weakly in Hilbert-Schmidt and $h_{\rm mf} \geq 0$, by Fatou's lemma we have

$$0 \leq \operatorname{Tr}(h_{\rm mf}\gamma_0) \leq \liminf_{\varepsilon \to 0^+} \operatorname{Tr}(h_{\rm mf}\gamma_\varepsilon) \to 0.$$

Thus $h_{\rm mf}\gamma_0 = 0$. Since $h_{\rm mf}$ has a unique ground state u_0, we have $\gamma_0 = \lambda |u_0\rangle\langle u_0|$ for some $\lambda \geq 0$. But we have proved that $\rho_{\gamma_0} = |u_0|^2$, hence $\lambda = 1$. Thus

$$\gamma_\varepsilon \rightharpoonup \gamma_0 = |u_0\rangle\langle u_0|$$

weakly in the Hilbert-Schmidt topology. Consequently,

$$\langle u_0, \gamma_\varepsilon u_0\rangle = \operatorname{Tr}\Big(|u_0\rangle\langle u_0|\gamma_\varepsilon\Big) \to 1.$$

This completes the proof. *q.e.d.*

Exercise. *Let $\{A_n\}_{n\geq 1}$ be a sequence Hilbert-Schmidt operators on $L^2(\mathbb{R}^d)$. Prove that $A_n \rightharpoonup A_0$ weakly in the Hilbert-Schmidt topology if and only if $A_n(\cdot,\cdot) \rightharpoonup A_0(\cdot,\cdot)$ weakly in $L^2(\mathbb{R}^d \times \mathbb{R}^d)$, where $A_n(x,y)$ is the kernel of A_n.*

Exercise. *Let $\{\gamma_n\}_{n\geq 1}$ be a sequence of Hilbert-Schmidt operators on $L^2(\mathbb{R}^d)$ such that $\gamma_n \geq 0$ and $\gamma_n \rightharpoonup \gamma_0$ weakly in the Hilbert-Schmidt topology. Prove that $\gamma_0 \geq 0$ and for any self-adjoint operator $A \geq 0$ on $L^2(\mathbb{R}^d)$, we have*

$$\operatorname{Tr}(A\gamma_0) \leq \liminf_{n\to\infty} \operatorname{Tr}(A\gamma_n).$$

Here $\operatorname{Tr}(A\gamma_n) := \operatorname{Tr}(A^{1/2}\gamma_n A^{1/2}) = \operatorname{Tr}(\gamma_n^{1/2} A \gamma_n^{1/2}) \in [0,\infty]$.

Exercise. *Let $\{\gamma_n\}_{n\geq 1}$ be a sequence of trace class operators on $L^2(\mathbb{R}^d)$ such that $\gamma_n \geq 0$,* $\operatorname{Tr}\gamma_n = 1$ *and*

$$\operatorname{Tr}((1-\Delta)^{1/2}\gamma_n(1-\Delta)^{1/2}) \leq C.$$

1. Prove that up to a subsequence, we have the weak convergence

$$(1-\Delta)^{1/2}\gamma_n(1-\Delta)^{1/2} \rightharpoonup (1-\Delta)^{1/2}\gamma_0(1-\Delta)^{1/2}$$

in the Hilbert-Schmidt topology, where $\gamma_0 \geq 0$ is a trace class operator on $L^2(\mathbb{R}^d)$.
2. Prove that

$$\lim_{n\to\infty}\int_{\mathbb{R}^d} U\rho_{\gamma_n} = \int_{\mathbb{R}^d} U\rho_{\gamma_0}, \quad \forall U \in C_c^\infty(\mathbb{R}^d).$$

Hint: If $d \leq 3$ you can show that $(1-\Delta)^{-1/2}U(1-\Delta)^{-1/2}$ is a Hilbert-Schmidt operator on $L^2(\mathbb{R}^d)$. For general case $d \geq 1$, you may use the weak- convergence in trace class.*

4.6 Short-range interactions

So far we have derived Hartree theory with regular interaction potentials. Now we consider the case of short-range potentials. Fix a constant $\beta > 0$ and consider the Hamiltonian

$$H_N = \sum_{i=1}^N(-\Delta_{x_i} + V(x_i)) + \frac{1}{N-1}\sum_{1\leq i<j\leq N} N^{d\beta}w(N^\beta(x_i - x_j))$$

on $L^2(\mathbb{R}^d)^{\otimes_s N}$. By restricting to the uncorrelated states $u^{\otimes N}$ and taking the formal limit

$$N^{d\beta}w(N^\beta x) \rightharpoonup b\delta_0(x), \quad b = \int_{\mathbb{R}^d} w$$

we obtain the Hartree/Gross-Pitaevskii functional

$$\mathcal{E}_{\rm GP}(u) = \int_{\mathbb{R}^d}\Big(|\nabla u(x)|^2 + V(x)|u(x)|^2 + \frac{b}{2}|u(x)|^4\Big).$$

We consider the ground state energy of H_N

$$E_N := \inf_{\|\Psi\|_{L^2(\mathbb{R}^d)^{\otimes_s N}}=1}\langle \Psi, H_N\Psi\rangle$$

and the Gross-Pitaevskii energy

$$e_{\rm GP} := \inf_{\|u\|_{L^2(\mathbb{R}^d)}=1}\mathcal{E}_{\rm GP}(u).$$

When $V(x) \to \infty$ as $|x| \to \infty$ and $b \geq 0$, $e_{\rm GP}$ has a unique minimizer (up to a phase) $u_0 \geq 0$ which solves the Gross-Pitaevskii equation

$$(-\Delta + V + b|u_0|^2 - \mu)u_0 = 0, \quad \mu \in \mathbb{R}.$$

Theorem (Convergence to Gross-Pitaevskii theory)**.** *Assume that*

- $0 \leq V \in L^\infty_{\rm loc}(\mathbb{R}^d), \quad \lim_{|x|\to\infty} V(x) = \infty,$
- $0 \leq w \in C_c^\infty(\mathbb{R}^d).$

Fix $1 \leq d \leq 3$ *and* $0 < \beta < 1/d$. *Then we have*

$$\lim_{N\to\infty} \frac{E_N}{N} = e_{\rm GP}.$$

Moreover, if Ψ_N *is an approximate ground state for* H_N, *namely* $\langle \Psi_N, H_N\Psi_N\rangle = Ne_{\rm GP} + o(N)$, *then we have the complete Bose-Einstein condensation*

$$\lim_{N\to\infty} \frac{\langle u_0, \gamma^{(1)}_{\Psi_N} u_0\rangle}{N} = 1.$$

Proof. **Step 1.** Denote $w_N(x) = N^{b\beta}w(N^\beta x)$ and define the N-dependent Hartree energy

$$e_{H,N} := \inf_{\|u\|_{L^2(\mathbb{R}^d)}=1} \mathcal{E}_{H,N}(u)$$

where

$$\mathcal{E}_{H,N}(u) := \int_{\mathbb{R}^d} \big(|\nabla u(x)|^2 + V(x)|u(x)|^2\big){\rm d}x + \frac{1}{2}\iint |u(x)|^2|u(y)|^2 w_N(x-y){\rm d}x{\rm d}y.$$

By the variational principle, we have the obvious upper bound

$$\frac{E_N}{N} \leq \inf_{\|u\|_{L^2}=1]} \frac{\langle u^{\otimes N}, H_N u^{\otimes N}\rangle}{N} \leq e_{H,N}.$$

Note that

$$\widehat{w_N}(k) = \int_{\mathbb{R}^d} w_N(x)e^{-i2\pi k\cdot x}{\rm d}x = \int_{\mathbb{R}^d} N^{d\beta}w(N^\beta x)e^{-i2\pi(N^{-\beta}k)\cdot(N^\beta x)}{\rm d}x$$

$$= \int_{\mathbb{R}^d} w(x) e^{-i2\pi(N^{-\beta}k)\cdot x} \mathrm{d}x = \widehat{w}(N^{-\beta}k).$$

Therefore, since $\widehat{w} \in L^1(\mathbb{R}^d)$ and $\beta < 1/d$ we have

$$\int_{\mathbb{R}^d} |\widehat{w_N}| = \int_{\mathbb{R}^d} |\widehat{w}(N^{-\beta}k)| \mathrm{d}k = N^{d\beta} \int_{\mathbb{R}^d} |\widehat{w}| = o(N).$$

Therefore, we can repeat the proof of the convergence to Hartree energy to obtain

$$\lim_{N\to\infty} \left| \frac{E_N}{N} - e_{H,N} \right| = 0.$$

Step 2. Next, we show that

$$\lim_{N\to\infty} e_{H,N} = e_{\mathrm{GP}}.$$

Since $w \geq 0$ by the Cauchy-Schwarz inequality we have

$$\begin{aligned} \iint |u(x)|^2 |u(y)|^2 w_N(x-y) \mathrm{d}x\mathrm{d}y &\leq \iint \frac{|u(x)|^4 + |u(y)|^4}{2} w_N(x-y) \\ &= \|w_N\|_{L^1} \int_{\mathbb{R}^d} |u|^4 = b \int_{\mathbb{R}^d} |u|^4. \end{aligned}$$

Therefore,

$$\mathcal{E}_{H,N}(u) \leq \mathcal{E}_{\mathrm{GP}}(u), \quad \forall u \in H^1(\mathbb{R}^d)$$

and hence by the variational principle we get the uniform upper bound

$$e_{H,N} \leq e_{\mathrm{GP}}, \quad \forall N.$$

Moreover,

$$\begin{aligned} \mathcal{E}_{\mathrm{GP}}(u) - \mathcal{E}_{H,N}(u) &= b \int_{\mathbb{R}^d} |u|^4 - \iint |u(x)|^2 |u(y)|^2 w_N(x-y) \mathrm{d}x\mathrm{d}y \\ &= \iint |u(x)|^4 w_N(x-y) \mathrm{d}x\mathrm{d}y - \iint |u(x)|^2 |u(y)|^2 w_N(x-y) \mathrm{d}x\mathrm{d}y \\ &= \iint |u(x)|^2 (|u(x)|^2 - |u(y)|^2) w_N(x-y) \mathrm{d}x\mathrm{d}y \end{aligned}$$

Using

$$\Big| |u(x)|^2 - |u(y)|^2 \Big| = \Big| \int_0^1 \frac{d}{dt} |u(y + t(x-y))|^2 \mathrm{d}t \Big|$$

$$\leq \int_0^1 2|u(y+t(x-y)||\nabla u(y+t(x-y))|.|x-y|\mathrm{d}t$$

and Hölder's inequality we find that

$$\begin{aligned}
&\Big|\mathcal{E}_{\rm GP}(u) - \mathcal{E}_{H,N}(u)\Big| \\
&\leq 2\int_0^1 \Big(\iint_{\mathbb{R}^d\times\mathbb{R}^d} |u(x)|^2 |u(y+t(x-y))||\nabla u(y+t(x-y))|.|x-y|w_N(x-y)\mathrm{d}x\mathrm{d}y\Big)dt \\
&= 2\int_0^1 \int_{\mathbb{R}^d} \Big(\int_{\mathbb{R}^d} |u(y+z)|^2 |u(y+tz)||\nabla u(y+tz)|\mathrm{d}y\Big)|z|w_N(z)\mathrm{d}z dt \\
&\leq 2\int_0^1 \int_{\mathbb{R}^d} \Big(\int_{\mathbb{R}^d} |u(y+z)|^6\mathrm{d}y\Big)^{1/3}\Big(\int_{\mathbb{R}^d} |u(y+tz)|^6\mathrm{d}y\Big)^{1/6}\Big(\int_{\mathbb{R}^d} |\nabla u(y+tz)|^2\mathrm{d}y\Big)^{1/2}|z|w_N(z)\mathrm{d}z\mathrm{d}t \\
&\leq 2\int_0^1 \|u\|_{L^6}^3 \|\nabla u\|_{L^2} \int_{\mathbb{R}^d} |z|w_N(z)\mathrm{d}z\mathrm{d}t \leq CN^{-\beta}\|u\|_{L^6}^3\|\nabla u\|_{L^2}
\end{aligned}$$

When $d \leq 3$, we have the Sobolev's embedding $H^1(\mathbb{R}^d) \subset L^6(\mathbb{R}^d)$, and hence

$$\Big|\mathcal{E}_{\rm GP}(u) - \mathcal{E}_{H,N}(u)\Big| \leq CN^{-\beta}\|u\|_{H^1}^4.$$

Now let u_N be a ground state for the Hartree problem $e_{H,N}$. Then $\|u_N\|_{L^2} = 1$. Moreover, using $V, w \geq 0$ we have

$$C \geq \mathcal{E}_{H,N}(u_N) \geq \int_{\mathbb{R}^d} |\nabla u_N|^2.$$

Thus $\{u_N\}_{N\geq 1}$ is bounded in $H^1(\mathbb{R}^d)$. Therefore,

$$\Big|\mathcal{E}_{\rm GP}(u_N) - \mathcal{E}_{H,N}(u_N)\Big| \leq CN^{-\beta}\|u_N\|_{H^1}^4 \to 0 \quad \text{as } N\to\infty.$$

Consequently,

$$e_{\rm GP} \leq \mathcal{E}_{\rm GP}(u_N) \leq \mathcal{E}_{H,N}(u_N) + o(1)_{N\to\infty} \leq e_{H,N} + o(1)_{N\to\infty}.$$

Thus we conclude that

$$\lim_{N\to\infty} e_{H,N} = e_{\rm GP}.$$

Combining with the result from Step 1, we obtain the energy convergence

$$\lim_{N\to\infty} \frac{E_N}{N} = e_{\rm GP}.$$

Step 3. Finally we prove the BEC. This can be done by the Hellmann-Feynman argument again. For any $\varepsilon > 0$, we define the perturbed Hamiltonian

$$H_{N,\varepsilon} = H_N + \varepsilon \sum_{i=1}^{N} P_{x_i}, \quad P = |u_0\rangle\langle u_0|$$

and call $E_{N,\varepsilon}$ the ground state energy of $H_{N,\varepsilon}$. Then following the above proof of

$$E_N = N e_{\mathrm{GP}} + o(N),$$

we also have

$$E_{N,\varepsilon} = N e_{\mathrm{GP},\varepsilon} + o(N)$$

where

$$e_{\mathrm{GP},\varepsilon} := \inf_{\substack{\gamma \geq 0 \text{ on } L^2(\mathbb{R}^d) \\ \operatorname{Tr}\gamma = 1}} \Big\{ \operatorname{Tr}((-\Delta + V + \varepsilon P)\gamma) + \frac{b}{2} \int_{\mathbb{R}^d} \rho_\gamma^2(x) \mathrm{d}x \Big\}.$$

Therefore, if Ψ_N is an approximate ground state for H_N, then by the variational principle, we have

$$\begin{aligned} \frac{\langle u_0, \gamma_{\Psi_N}^{(1)} u_0 \rangle}{N} &= \frac{1}{N} \langle \Psi_N, \sum_{i=1}^{N} P_i \Psi_N \rangle = \frac{1}{\varepsilon N} \Big(\langle \Psi_N, \sum_{i=1}^{N} H_{N,\varepsilon} \Psi_N \rangle - \langle \Psi_N, H_N \Psi_N \rangle \Big) \\ &\geq \frac{1}{\varepsilon N} \Big(E_{N,\varepsilon} - E_N + o(N) \Big) = \frac{1}{\varepsilon N} \Big(N e_{\mathrm{GP},\varepsilon} - N e_{\mathrm{GP}} + o(N) \Big) \to_{N \to \infty} \frac{e_{\mathrm{GP},\varepsilon} - e_{\mathrm{GP}}}{\varepsilon}. \end{aligned}$$

Thus to obtain the complete BEC it remains to show that

$$\lim_{\varepsilon \to 0^+} \frac{e_{\mathrm{GP},\varepsilon} - e_{\mathrm{GP}}}{\varepsilon} = 1.$$

Since $\varepsilon \operatorname{Tr}(P\gamma) \leq \varepsilon$ we get the uniform upper bound

$$\frac{e_{\mathrm{GP},\varepsilon} - e_{\mathrm{GP}}}{\varepsilon} \leq 1.$$

For the lower bound, let γ_ε be an approximate minimizer for $e_{\mathrm{GP},\varepsilon}$, namely

$$\operatorname{Tr}((-\Delta + V + \varepsilon P)\gamma_\varepsilon) + \frac{b}{2} \int_{\mathbb{R}^d} \rho_{\gamma_\varepsilon}^2(x) \mathrm{d}x = e_{\mathrm{GP},\varepsilon} + o(\varepsilon).$$

Then using $\operatorname{Tr}(P\gamma) \geq 0$ and the Hoffmann–Ostenhof inequality we get

$$\mathcal{E}_{\mathrm{GP}}(\sqrt{\rho_{\gamma_\varepsilon}}) \leq e_{\mathrm{GP},\varepsilon} + o(\varepsilon) \leq e_{\mathrm{GP}} + O(\varepsilon).$$

Thus $\sqrt{\rho_{\gamma_\varepsilon}}$ is a minimizing sequence for $e_{\rm GP}$, and hence we deduce that $\sqrt{\rho_{\gamma_\varepsilon}} \to u_0$ strongly in $L^2(\mathbb{R}^d)$. Since $\sqrt{\rho_{\gamma_\varepsilon}}$ is bounded in $H^1(\mathbb{R}^d)$, by Sobolev's embedding theorem we get $\sqrt{\rho_{\gamma_\varepsilon}} \to u_0$ strongly in $L^p(\mathbb{R}^d)$ for all $p \in [2, 2^*)$. When $d \leq 3$, we get $2^* \geq 6 > 4$, and hence

$$\int_{\mathbb{R}^d} (\rho_{\gamma_\varepsilon} - |u_0|^2)^2 \to 0,$$

which is equivalent to

$$\begin{aligned}\frac{b}{2}\int_{\mathbb{R}^d} \rho_{\gamma_\varepsilon}^2(x){\rm d}x &= b\int_{\mathbb{R}^d} \rho_{\gamma_\varepsilon}(x)|u_0(x)|^2{\rm d}x - \frac{b}{2}\int_{\mathbb{R}^d}|u_0(x)|^4{\rm d}x + o(1)_{\varepsilon\to 0}\\ &= b\,{\rm Tr}(|u_0|^2\gamma_\varepsilon) + e_{\rm GP} - \mu\end{aligned}$$

Here $\mu \in \mathbb{R}$ is the chemical potential in the GP equation

$$(-\Delta + V + b|u_0|^2 - \mu)u_0 = 0.$$

Thus we find that

$$\begin{aligned}e_{{\rm GP},\varepsilon} + o(\varepsilon) &= {\rm Tr}((-\Delta + V + \varepsilon P)\gamma_\varepsilon) + \frac{b}{2}\int_{\mathbb{R}^d}\rho_{\gamma_\varepsilon}^2(x){\rm d}x\\ &= {\rm Tr}((-\Delta + V + b|u_0|^2 - \mu)\gamma_\varepsilon) + e_{\rm GP} + o(1)_{\varepsilon\to 0}.\end{aligned}$$

Since we have prove $e_{{\rm GP},\varepsilon} \to e_{\rm GP}$, we get

$${\rm Tr}((-\Delta + V + b|u_0|^2 - \mu)\gamma_\varepsilon) \to 0.$$

Note that u_0 is the unique ground state of the operator

$$h = -\Delta + V + b|u_0|^2 - \mu.$$

Moreover, since $V(x) \to \infty$ as $|x| \to \infty$, h has compact resolvent. Thus h has eigenvalues

$$0 = \lambda_1(h) < \lambda_2(h) \leq ...$$

Using the spectral gap $\lambda_2(h) > \lambda_1(h)$, we conclude that

$${\rm Tr}(P\gamma_\varepsilon) \to 1.$$

Thus

$$\begin{aligned} e_{\mathrm{GP},\varepsilon} + o(\varepsilon) &= \mathrm{Tr}((-\Delta + V + \varepsilon P)\gamma_\varepsilon) + \frac{b}{2}\int_{\mathbb{R}^d} \rho^2_{\gamma_\varepsilon}(x)\mathrm{d}x \\ &\geq \mathrm{Tr}((-\Delta + V)\gamma_\varepsilon) + \frac{b}{2}\int_{\mathbb{R}^d} \rho^2_{\gamma_\varepsilon}(x)\mathrm{d}x + \varepsilon \\ &\geq \mathcal{E}_{\mathrm{GP}}(\sqrt{\rho_{\gamma_\varepsilon}}) + \varepsilon \geq e_{\mathrm{GP}} + \varepsilon \end{aligned}$$

which gives the desired lower bound

$$\liminf_{\varepsilon \to 0^+} \frac{e_{\mathrm{GP},\varepsilon} - e_{\mathrm{GP}}}{\varepsilon} \geq 1.$$

This completes the proof of the BEC. *q.e.d.*

Remarks:

- The same result holds true for all $0 < \beta < \infty$ if $d = 1, 2$ and all $0 < \beta < 1$ if $d = 3$, but the proof is more complicated. The case $\beta > 1/d$ is interesting because in this case, the range of the interaction potential $N^{-\beta}$ is much smaller than the mean-distance between particles $N^{-1/d}$. This is called the **dilute regime**. In contrast, when $\beta < 1/d$, then the range of the interaction potential $N^{-\beta}$ is much bigger than the mean-distance between particles $N^{-1/d}$, and hence each particle interacts with many others. This is the reason why the case $\beta < 1/d$ is easier to justify the mean-field approximation (which is somewhat similar to **the law of large numbers** in probability theory).

- In the case $d = 3$ and $\beta = 1$, the result is still correct provided that in the Gross-Pitaevskii functional

$$\mathcal{E}_{\mathrm{GP}}(u) = \int_{\mathbb{R}^d} \Big(|\nabla u(x)|^2 + V(x)|u(x)|^2 + \frac{b}{2}|u(x)|^2 \Big).$$

 the constant b is not $\int w$ but rather given by the **scattering energy** of w

$$b := \inf \left\{ \int_{\mathbb{R}^3} 2|\nabla f|^2 + w|f|^2, \quad \lim_{|x|\to\infty} f(x) = 1 \right\}.$$

 This variational problem has a unique minimizer $0 \leq f \leq 1$ and it solves the **zero-scattering equation**

$$(-2\Delta + w)f = 0.$$

Moreover, we have

$$f(x) = 1 - \frac{a}{|x|} + o(|x|^{-1})_{|x|\to\infty}$$

and

$$a = \frac{1}{8\pi} b$$

is called the **scattering length** of w. If w is the **hard sphere potential** of $B(0, R)$, then $a = R$. In general, we have **Born's series**

$$b = 8\pi a = \int_{\mathbb{R}^3} wf = \int_{\mathbb{R}^3} w - \int_{\mathbb{R}^3} w(-2\Delta + w)^{-1} w = ...$$

Thus $\frac{1}{8\pi} \int w$ is the first Born's approximation for the scattering length (it is $> a$ except when $w \equiv 0$). By scaling, the scattering length of $N^2 w(N\cdot)$ is a/N. The derivation of the GP theory in this critical case is significantly more difficult. We will come back to this problem later when we have more tools from the **Fock space formalism** and **Bogoliubov's approximation**.

Chapter 5

Fock space formalism

Definition. *Let $\mathscr{H}$ be a one-particle Hilbert space. The* **bosonic Fock space** *associated to $\mathscr{H}$ is the Hilbert space*

$$\mathcal{F} = \mathcal{F}(\mathscr{H}) = \bigoplus_{n=0}^{\infty} \mathscr{H}^{\otimes_s n} = \mathbb{C} \oplus \mathscr{H} \oplus \mathscr{H}^{\otimes s2} \oplus ...$$

- *Any vector in $\mathcal{F}$ has the form $\Psi = (\Psi_n)_{n=0}^{\infty}$ where $\Psi_n \in \mathscr{H}^{\otimes_s n}$ and*

$$\|\Psi\|_{\mathcal{F}}^2 = \sum_{n=0}^{\infty} \|\Psi_n\|_{\mathscr{H}^{\otimes_s n}}^2$$

- *The vector $\Omega = (1, 0, 0, ...)$ is called the* **vacuum**.

- *The expectation of the number of particles in the state $\Psi = (\Psi_n)_{n=0}^{\infty} \in \mathcal{F}$ is*

$$\sum_{n=0}^{\infty} n \|\Psi_n\|_{\mathscr{H}^{\otimes_s n}}^2 .$$

  This is the same to $\langle \Psi, \mathcal{N} \Psi \rangle$ where

$$\mathcal{N} := \sum_{n=0}^{\infty} n \mathbb{1}_{\mathscr{H}^{\otimes sn}}$$

  is called the **number operator**. *In particular, $\langle \Omega, \mathcal{N} \Omega \rangle = 0$.*

5.1 Creation and annihilation operators

Definition. *Let $\mathscr{H}$ be a one-particle Hilbert space and let $\mathcal{F} = \mathcal{F}(\mathscr{H})$ be the bosonic Fock space. For any $f \in \mathscr{H}$ we can define the* **creation operator** *$a^*(f)$ and the* **annihilation operator** *$a(f)$ on $\mathcal{F}$ as follows:*

- *$a^*(f) : \mathscr{H}^{\otimes_s n} \to \mathscr{H}^{\otimes_s n+1}$ for all $n = 0, 1, 2, ...$*

$$(a^*(f)\Psi_n)(x_1, \dots, x_{n+1}) = \frac{1}{\sqrt{n+1}} \sum_{j=1}^{n+1} f(x_j)\Psi_n(x_1, \dots, x_{j-1}, x_{j+1}, \dots, x_{n+1}).$$

- *$a(f) : \mathscr{H}^{\otimes_s n} \to \mathscr{H}^{\otimes_s n-1}$ for all $n = 0, 1, 2, ...$ (with convention $\mathscr{H}^{\otimes_s -1} = \{0\}$)*

$$(a(f)\Psi_n)(x_1, \dots, x_{n-1}) = \sqrt{n} \int \overline{f(x_n)}\Psi(x_1, \dots, x_n)\mathrm{d}x_n.$$

Here we think of $\mathscr{H} \subset L^2(\mathbb{R}^d)$ to simplify the notation.

Remarks:

- $a^*(f)\Omega = f$ and $a(f)\Omega = 0$.
- $f \mapsto a^*(f)$ is **linear**, but $f \mapsto a(f)$ is **anti-llinear**.

Example: If $\mathscr{H}$ is one-dimensional, $\mathscr{H} = \mathrm{span}\{f\}$, $\|f\| = 1$. Then $\mathcal{F}(\mathscr{H})$ has an orthonormal basis $\{|n\rangle\}_{n=0,1,2,...}$ where

$$|0\rangle = (1, 0, 0, ...) = \Omega, \quad |1\rangle = (0, f, 0, ...), \quad |2\rangle = (0, 0, f^{\otimes 2}, 0, ...), \quad |n\rangle = (0, ..., f^{\otimes n}, 0, ...)$$

In this case,

$$a^*(f)|n\rangle = \sqrt{n+1}|n+1\rangle, \quad n \geq 0$$
$$a(f)|n\rangle = \sqrt{n}|n-1\rangle, \quad \forall n \geq 1.$$

Exercise. *This problem allows us to think of $L^2(\mathbb{R})$ as the Fock space $\mathcal{F}(\mathbb{C})$. Define the operators a and a^+ on $L^2(\mathbb{R})$ by*

$$a = \frac{1}{\sqrt{2}}\Big(x + \frac{d}{dx}\Big), \quad a^* = \frac{1}{\sqrt{2}}\Big(x - \frac{d}{dx}\Big).$$

Define the functions $\{f_n\}_{n\geq 0} \subset L^2(\mathbb{R})$ by

$$f_0(x) = \pi^{-1/4} e^{-|x|^2/2}, \quad f_{n+1} = \frac{a^* f_n}{\sqrt{n+1}}, \quad \forall n \geq 0.$$

1. *Prove that $[a, a^*] = 1$ (identity).*
2. *Prove that $af_0 = 0$ and $af_{n+1} = \sqrt{n+1} f_n$ for all $n \geq 0$.*
3. *Prove that $\{f_n\}_{n\geq 0}$ is an orthonormal basis for $L^2(\mathbb{R})$.*

Hint: You can use the fact that $\mathrm{Span}\{p(x)e^{-x^2/2} \,|\, p(x) \text{ is a polynomial}\}$ *is dense in $L^2(\mathbb{R})$.*

Exercise. *Consider the Fock space $\mathcal{F}(\mathscr{H})$. Prove that for all $f \in \mathscr{H}$, we have*

$$\|a(f)\Psi\|_{\mathcal{F}} \leq \|f\|_{\mathscr{H}} \|\mathcal{N}^{1/2}\Psi\|, \quad \forall \Psi \in Q(\mathcal{N}).$$

Here $Q(\mathcal{N})$ is the quadratic form domain for the number operator $\mathcal{N}$.

Exercise. *Consider the Fock space $\mathcal{F}(\mathscr{H})$. Prove that for all $f \in \mathscr{H}$, $a(f)$ and $a^*(f)$ are adjoints, namely*

$$\langle a(f)\Psi, \Phi\rangle_{\mathcal{F}} = \langle \Psi, a^*(f)\Phi\rangle_{\mathcal{F}}, \quad \forall \Psi, \Phi \in Q(\mathcal{N}).$$

Theorem (Canonical Commutation Relations - CCR)**.** *Consider the Fock space $\mathcal{F}(\mathscr{H})$. For all $f, g \in \mathscr{H}$, we have*

$$[a(f), a(g)] = 0, \quad [a^*(f), a^*(g)] = 0, \quad [a(f), a^*(g)] = \langle f, g\rangle_{\mathscr{H}}.$$

Here $[A, B] := AB - BA$.

Proof. We may think of $\mathscr{H} \subset L^2(\mathbb{R}^d)$ for simplicity.

Step 1. First, let us prove that $[a(f), a(g)] = 0$, namely

$$a(f)a(g) = a(g)a(f).$$

It suffices to show that

$$a(f)a(g)\Psi_n = a(g)a(f)\Psi_n$$

for any function $\Psi_n \in \mathscr{H}^{\otimes_s n}$ and for any $n \geq 2$. By the definition of the annihilation operator, we have

$$\begin{aligned}
&(a(f)a(g)\Psi_n)(x_1, ..., x_{n-2}) = (a(f)(a(g)\Psi_n))(x_1, ..., x_{n-2}) \\
&= \Big(a(f)\Big[(y_1, ..., y_{n-1}) \mapsto \sqrt{n}\int \overline{g(x_n)}\Psi_N(y_1, ..., y_{n-1}, x_n)\mathrm{d}x_n\Big]\Big)(x_1, ..., x_{n-2}) \\
&= \sqrt{n}\sqrt{n-1}\int \overline{f(x_{n-1})}\Big(\int \overline{g(x_n)}\Psi_n(x_1, ..., x_{n-1}, x_n)\mathrm{d}x_n\Big)dx_{n-1} \\
&= \sqrt{n(n-1)}\iint \overline{f(x_{n-1})g(x_n)}\Psi_n(x_1, ..., x_{n-1}, x_n)dx_{n-1}dx_n.
\end{aligned}$$

Using Fubini's theorem and the bosonic symmetry

$$\Psi_n(x_1, ..., x_{n-1}, x_n) = \Psi_n(x_1, ..., x_n, x_{n-1})$$

we can write

$$\begin{aligned}
(a(g)a(f)\Psi_n)(x_1, ..., x_{n-2}) &= \sqrt{n(n-1)}\iint \overline{g(x_{n-1})f(x_n)}\Psi_n(x_1, ..., x_{n-1}, x_n)dx_{n-1}dx_n \\
&= \sqrt{n(n-1)}\iint \overline{g(x_n)f(x_{n-1})}\Psi_n(x_1, ..., x_n, x_{n-1})dx_{n-1}dx_n \\
&= \sqrt{n(n-1)}\iint \overline{g(x_n)f(x_{n-1})}\Psi_n(x_1, ..., x_{n-1}, x_n)dx_{n-1}dx_n \\
&= (a(f)a(g)\Psi_n)(x_1, ..., x_{n-2}).
\end{aligned}$$

Thus $a(f)a(g) = a(g)a(f)$.

Step 2. Since $a^*(f)$ is the adjoint of $a(f)$, using $[a(f), a(g)] = 0$ we have

$$0 = ([a(f), a(g)])^* = (a(f)a(g) - a(g)a(f))^* = (a^*(g)a^*(f) - a^*(f)a^*(g)) = -[a^*(f), a^*(g)].$$

Thus $[a^*(f), a^*(g)] = 0$.

Step 3. Finally, we prove that

$$[a(f), a^*(g)] = a(f)a^*(g) - a^*(g)a(f) = \langle f, g\rangle.$$

When testing with the vacuum, we have

$$a(f)a^*(g)\Omega - a^*(g)a(f)\Omega = a(f)g - 0 = \langle f, g\rangle.$$

Now consider any function $\Psi_n \in \mathscr{H}^{\otimes_s n}$ with any $n \geq 1$. We have

$$\begin{aligned}
&(a(f)a^*(g)\Psi_n)(x_1, ..., x_n) = \Big(a(f)(a^*(g)\Psi_n)\Big)(x_1, ..., x_n) \\
&= \Big(a(f)\frac{1}{\sqrt{n+1}}\sum_{i=1}^{n+1} g(y_i)\Psi_n(y_1, ..., y_{i-1}, y_{i+1}, ..., y_{n+1})\Big)(x_1, ..., x_n) \\
&= \int \overline{f(x_{n+1})}\sum_{i=1}^{n+1} g(x_i)\Psi_n(x_1, ..., x_{i-1}, x_{i+1}, ..., x_{n+1})\mathrm{d}x_{n+1} \\
&= \langle f, g\rangle\Psi_n(x_1, ..., x_n) + \sum_{i=1}^{n} g(x_i)\int \overline{f(x_{n+1})}\Psi_n(x_1, ..., x_{i-1}, x_{i+1}, ..., x_{n+1})\mathrm{d}x_{n+1}.
\end{aligned}$$

On the other hand,

$$\begin{aligned}
&(a^*(g)a(f)\Psi_n)(x_1, ..., x_n) = \Big(a^*(g)(a(f)\Psi_n)\Big)(x_1, ..., x_n) \\
&= \Big(a^*(g)\sqrt{n}\int \overline{f(y_n)}\Psi_n(y_1, ..., y_n)\mathrm{d}y_n\Big)(x_1, ..., x_n) \\
&= \sum_{i=1}^{n} g(x_i)\int \overline{f(y_n)}\Psi_n(x_1, ..., x_{i-1}, x_{i+1}, ..., x_n, y_n)\mathrm{d}y_n \\
&= \sum_{i=1}^{n} g(x_i)\int \overline{f(x_{n+1})}\Psi_n(x_1, ..., x_{i-1}, x_{i+1}, ..., x_n, x_{n+1})\mathrm{d}x_{n+1}.
\end{aligned}$$

Here in the last identity we simply "renamed" y_n to x_{n+1}. Thus

$$a(f)a^*(g)\Psi_n - a^*(g)a(f)\Psi_n = \langle f, g\rangle\Psi_n(x_1, ..., x_n)$$

for all $\Psi_n \in \mathscr{H}^{\otimes_s n}$. This means

$$[a(f), a^*(g)] = a(f)a^*(g) - a^*(g)a(f) = \langle f, g\rangle.$$

q.e.d.

Exercise. *Assume that* $\mathscr{H}$ *has an orthonormal basis* $\{u_n\}_{n\geq 1}$. *Let* $a_n = a(u_n)$ *on the bosonic Fock space* $\mathcal{F}(\mathscr{H})$. *Prove that* $\mathcal{F}(\mathscr{H})$ *has an orthonormal basis with vectors*

$$|n_1, n_2, ...\rangle := (n_1! n_2! ...)^{-1/2} (a_1^*)^{n_1} (a_2^*)^{n_2} ... \Omega.$$

Here $n_1, n_2, ... \in \{0, 1, 2, ...\}$ *and there are only finitely many of* $\{n_k\}$ *are non-zero.*

Remark: Sometimes it is also convenient to write $|0\rangle = \Omega$.

5.2 Second quantization

Using the creation and annihilation operators, we can represent many operators on Fock space in a convenient way.

Theorem (Second quantization of one-body operators)**.** *Let* h *be a self-adjoint operator on the one-body Hilbert space* $\mathscr{H}$. *Then the operator on the bosonic Fock space* $\mathcal{F}(\mathscr{H})$

$$\mathrm{d}\Gamma(h) := \bigoplus_{n=0}^{\infty} \Big(\sum_{i=1}^{n} h_i \Big) = 0 \oplus h \oplus (h \otimes \mathbb{1} + \mathbb{1} \otimes h) \oplus ...$$

is called **the second quantization of** h. *It can be rewritten as*

$$\mathrm{d}\Gamma(h) = \sum_{m,n\geq 1} \langle u_m, h u_n \rangle a_m^* a_n.$$

Here $\{u_n\}_{n\geq 1}$ *is an orthogonal basis for* $\mathscr{H}$ *and* $a_n = a(u_n)$. *The representation is* **independent of the choice of the basis** *(provided that all* $\langle u_m, h u_n\rangle$ *are finite). The identity can be made rigorous at least on the domain*

$$\bigcup_{M=1}^{\infty} \bigoplus_{N=0}^{M} D(h_1 + ... + h_N) \subset \mathcal{F}.$$

Example: When $h = \mathbb{1}$ (the identity) we obtain the number operator

$$\mathcal{N} = \mathrm{d}\Gamma(1) = \sum_{m,n\geq 1} \langle u_m, u_n \rangle a_m^* a_n = \sum_{m,n\geq 1} \delta_{m=n} a_m^* a_n = \sum_{n\geq 1} a_n^* a_n.$$

Proof. It suffices to prove that

$$\sum_{i=1}^{N} h_i \Psi_N = \sum_{m,n\geq 1} \langle u_m, hu_n\rangle a_m^* a_n \Psi_N$$

for all $\Psi_N \in \mathscr{H}^{\otimes_s N}$ and for all N. Recall from a previous computation

$$(a_m^* a_n \Psi_N)(x_1,...,x_N) = \sum_{i=1}^{N} u_m(x_i) \int \overline{u_n(y)} \Psi_n(x_1,...,x_{i-1},x_{i+1},...,x_N,y)\mathrm{d}y.$$

Therefore,

$$\begin{aligned}
&\sum_{m,n} \langle u_m, hu_n\rangle (a_m^* a_n \Psi_N)(x_1,...,x_N) \\
&= \sum_{m,n} \langle u_m, hu_n\rangle \sum_{i=1}^{N} u_m(x_i) \int \overline{u_n(y)} \Psi_N(x_1,...,x_{i-1},x_{i+1},...,x_N,y)\mathrm{d}y \\
&= \sum_{i=1}^{N} \sum_{n} \Big(\sum_{m} \langle u_m, hu_n\rangle u_m(x_i) \Big) \int \overline{u_n(y)} \Psi_N(x_1,...,x_{i-1},x_{i+1},...,x_N,y)\mathrm{d}y \\
&= \sum_{i=1}^{N} \sum_{n} (hu_n)(x_i) \int \overline{u_n(y)} \Psi_N(x_1,...,x_{i-1},x_{i+1},...,x_N,y)\mathrm{d}y \\
&= \sum_{i=1}^{N} \sum_{n} \Big[(|hu_n\rangle\langle u_n|)_{x_i} \Psi_N \Big] (x_1,...,x_{i-1},x_i,x_{i+1},...,x_N) \\
&= \sum_{i=1}^{N} \Big[\Big(h \sum_{n} |u_n\rangle\langle u_n| \Big)_{x_i} \Psi_N \Big] (x_1,...,x_{i-1},x_i,x_{i+1},...,x_N) \\
&= \sum_{i=1}^{N} \Big[h_i \Psi_N \Big] (x_1,...,x_N).
\end{aligned}$$

Here we have used the Parseval's identity

$$\sum_{m} \langle u_m, hu_n\rangle u_m = hu_n$$

and the the resolution of the identity operator

$$\sum_{n} |u_n\rangle\langle u_n| = \mathbb{1}$$

(both use the fact that $\{u_n\}$ is an orthonormal basis for $\mathscr{H}$). This completes the proof.

q.e.d.

Theorem (Second quantization of two-body operators)**.** *Let W be a self-adjoint operator on $\mathscr{H}^{\otimes 2}$ such that $W_{12} = W_{21}$. Then the operator on the bosonic Fock space $\mathcal{F}(\mathscr{H})$*

$$\bigoplus_{n=0}^{\infty}\Big(\sum_{1\le i<j\le n} W_{ij}\Big) = 0\oplus 0\oplus W\oplus (W_{12}+W_{23}+W_{13})\oplus \ldots$$

is called **the second quantization of** W*. It can be rewritten as*

$$\bigoplus_{n=0}^{\infty}\Big(\sum_{1\le i<j\le n} W_{ij}\Big) = \frac{1}{2}\sum_{m,n,p,q\ge 1}\langle u_m\otimes u_n, W u_p\otimes u_q\rangle_{\mathscr{H}^{\otimes 2}} \quad a_m^* a_n^* a_p a_q$$

Here $\{u_n\}_{n\ge 1}$ is an orthogonal basis for $\mathscr{H}$ and $a_n = a(u_n)$. The representation is **independent of the choice of the basis**.

Proof. It suffices to prove that

$$2\Big\langle \Phi_N, \sum_{1\le i<j\le N} W_{ij}\Psi_N\Big\rangle = \Big\langle \Phi_N, \sum_{m,n,p,q}\langle u_m\otimes u_n, W u_p\otimes u_q\rangle a_m^* a_n^* a_p a_q \Psi_N\Big\rangle$$

for all $\Phi_N, \Psi_N \in \mathscr{H}^{\otimes_s N}$ and for all N. Recall from a previous computation

$$(a(f)a(g)\Psi_N)(x_1,\ldots,x_{N-2}) = \sqrt{N(N-1)}\iint \overline{f(y)g(z)}\Psi_N(x_1,\ldots,x_{N-2},y,z)\mathrm{d}y\mathrm{d}z.$$

Therefore,

$$\begin{aligned}
&\Big\langle \Phi_N, \sum_{m,n,p,q}\langle u_m\otimes u_n, W u_p\otimes u_q\rangle a_m^* a_n^* a_p a_q \Psi_N\Big\rangle \\
&= \sum_{m,n,p,q}\langle u_m\otimes u_n, W u_p\otimes u_q\rangle \Big\langle a_m a_n \Phi_N, a_p a_q \Psi_N\Big\rangle \\
&= \sum_{m,n,p,q}\langle u_m\otimes u_n, W u_p\otimes u_q\rangle \int \overline{(a_m a_n\Phi_N)(x_1,\ldots,x_{N-2})}(a_p a_q\Psi_N)(x_1,\ldots,x_{N-2})\mathrm{d}x_1\ldots\mathrm{d}x_{N-2} \\
&= \sum_{m,n,p,q}\langle u_m\otimes u_n, W u_p\otimes u_q\rangle \int \overline{\Big(\sqrt{N(N-1)}\iint \overline{u_m(y')u_n(z')}\Phi_N(x_1,\ldots,x_{N-2},y',z')\mathrm{d}y'\mathrm{d}z'\Big)}\times \\
&\quad\times\Big(\sqrt{N(N-1)}\iint \overline{u_p(y)u_q(z)}\Psi_N(x_1,\ldots,x_{N-2},y,z)\mathrm{d}y\mathrm{d}z\Big)\mathrm{d}x_1\ldots\mathrm{d}x_{N-2} \\
&= N(N-1)\sum_{m,n,p,q}\langle u_m\otimes u_n, W u_p\otimes u_q\rangle \int u_m(y')u_n(z')\overline{u_p(y)u_q(z)}\times
\end{aligned}$$

$$\times \overline{\Phi_N(x_1, ..., x_{N-2}, y', z')}\Psi_N(x_1, ..., x_{N-2}, y, z)\mathrm{d}x_1...\mathrm{d}x_{N-2}\mathrm{d}y\mathrm{d}y'\mathrm{d}z\mathrm{d}z'$$

Since $\{u_m \otimes u_m\}_{m,n}$ is an orthonormal basis for $\mathscr{H}^{\otimes 2}$, we can use Parseval's identity to get

$$\sum_{m,n} \langle u_m \otimes u_n, W u_p \otimes u_q \rangle u_m \otimes u_n = W u_p \otimes u_q.$$

Therefore,

$$\begin{aligned}
&\Big\langle \Phi_N, \sum_{m,n,p,q} \langle u_m \otimes u_n, W u_p \otimes u_q \rangle a_m^* a_n^* a_p a_q \Psi_N \Big\rangle \\
&= N(N-1) \int \sum_{m,n,p,q} \langle u_m \otimes u_n, W u_p \otimes u_q \rangle (u_m \otimes u_n)(y', z') \overline{u_p(y) u_q(z)} \times \\
&\quad \times \overline{\Phi_N(x_1, ..., x_{N-2}, y', z')}\Psi_N(x_1, ..., x_{N-2}, y, z)\mathrm{d}x_1...\mathrm{d}x_{N-2}\mathrm{d}y\mathrm{d}y'\mathrm{d}z\mathrm{d}z' \\
&= N(N-1) \int \sum_{p,q} (W u_p \otimes u_q)(y', z') \overline{u_p(y) u_q(z)} \times \\
&\quad \times \overline{\Phi_N(x_1, ..., x_{N-2}, y', z')}\Psi_N(x_1, ..., x_{N-2}, y, z)\mathrm{d}x_1...\mathrm{d}x_{N-2}\mathrm{d}y\mathrm{d}y'\mathrm{d}z\mathrm{d}z' \\
&= N(N-1) \sum_{p,q} \Big\langle \Phi_N, \Big(W |u_p \otimes u_q\rangle\langle u_p \otimes u_q| \Big)_{x_{N-1}, x_N} \Psi_N \Big\rangle_{x_1, ..., x_N} \\
&= N(N-1) \Big\langle \Phi_N, W_{N-1,N} \Psi_N \Big\rangle = 2 \Big\langle \Phi_N, \sum_{1 \le i < j \le N} W_{i,j} \Psi_N \Big\rangle.
\end{aligned}$$

Here we have used

$$\sum_{p,q} |u_p \otimes u_q\rangle\langle u_p \otimes u_q| = \mathbb{1}_{\mathscr{H}^{\otimes 2}}$$

because $\{u_p \otimes u_q\}_{p,q}$ is an orthonormal basis for $\mathscr{H}^{\otimes 2}$. Thus we conclude that

$$\Big\langle \Phi_N, \sum_{m,n,p,q} \langle u_m \otimes u_n, W u_p \otimes u_q \rangle a_m^* a_n^* a_p a_q \Psi_N \Big\rangle = 2 \Big\langle \Phi_N, \sum_{1 \le i < j \le N} W_{i,j} \Psi_N \Big\rangle.$$

for all $\Phi_N, \Psi_N \in \mathscr{H}^{\otimes_s N}$, and for all N. This completes the proof. *q.e.d.*

Remarks:

- From the method of second quantization, the typical Hamiltonian

$$H_N = \sum_{i=1}^{N} h_i + \sum_{1 \le i < j \le N} W_{ij}$$

on $\mathscr{H}^{\otimes_s N}$ can be extended to be an operator on the bosonic Fock space $\mathcal{F}(\mathscr{H})$ as

$$\bigoplus_{N=0}^{\infty} H_N = \sum_{m,n} h_{mn} a_m^* a_n + \frac{1}{2} \sum_{m,n,p,q} W_{mnpq} a_m^* a_n^* a_p a_q$$

where $a_n = a(u_n)$ with an orthonormal basis $\{u_n\}$ for $\mathscr{H}$ and

$$h_{mn} = \langle u_m, h u_n \rangle_{\mathscr{H}}, \quad W_{mnpq} = \langle u_m \otimes u_n, W u_p \otimes u_q \rangle_{\mathscr{H}^{\otimes 2}}.$$

- In the littérature, when $\mathscr{H} \subset L^2(\mathbb{R}^d)$ people also use the creation and annihilation operators a_x^* and a_x, defined by

$$a^*(f) = \int f(x) a_x^* \mathrm{d}x, \quad a(f) = \int \overline{f(x)} a_x \mathrm{d}x, \quad \forall f \in \mathscr{H}.$$

These operator-valued distributions satisfy the CCR

$$[a_x, a_y] = 0, \quad [a_x^*, a_y^*] = 0, \quad [a_x, a_y^*] = \delta_0(x - y).$$

The advantage of these notations is that we can use the second quantization without specifying an orthonormal basis for $\mathscr{H}$. For example, the typical Hamiltonian

$$H_N = \sum_{i=1}^{N} (-\Delta_{x_i} + V(x_i)) + \sum_{1 \le i < j \le N} W(x_i - x_j)$$

on $L^2(\mathbb{R}^d)^{\otimes_s N}$ can be extended to be an operator on Fock space as

$$\bigoplus_{N=0}^{\infty} H_N = \int_{\mathbb{R}^d} a_x^* (-\Delta_x + V(x)) a_x \mathrm{d}x + \frac{1}{2} \iint W(x - y) a_x^* a_y^* a_x a_y \mathrm{d}x\mathrm{d}y.$$

5.3 Generalized one-body density matrices

Definition. *Let Ψ be a normalized vector in the bosonic Fock space $\mathcal{F}(\mathscr{H})$. Assume that $\Psi \in Q(\mathcal{N})$, namely $\langle \Psi, \mathcal{N} \Psi \rangle < \infty$. We define the* **one-body density matrix**

$\gamma_\Psi : \mathscr{H} \to \mathscr{H}$ *by*

$$\langle g, \gamma_\Psi f\rangle_{\mathscr{H}} = \langle \Psi, a^*(f)a(g)\Psi\rangle, \quad \forall f, g \in \mathscr{H}.$$

Exercise. *Let* Ψ *be a normalized vector in the bosonic Fock space* $\mathcal{F}(\mathscr{H})$ *with* $\langle \Psi, \mathcal{N}\Psi\rangle < \infty$. *Prove that the one-body density matrix* γ_Ψ *is a non-negative, trace class operator and*

$$\operatorname{Tr}\gamma_\Psi = \langle \Psi, \mathcal{N}\Psi\rangle < \infty.$$

Exercise. *Let a normalized vector* $\Psi \in \mathscr{H}^{\otimes_s N} \subset \mathcal{F}(\mathscr{H})$ *with* $\mathscr{H} = L^2(\mathbb{R}^d)$. *Prove that the one-body density matrix* γ_Ψ *defined by*

$$\langle g, \gamma_\Psi f\rangle_{\mathscr{H}} = \langle \Psi, a^*(f)a(g)\Psi\rangle, \quad \forall f, g \in \mathscr{H}$$

is **the same** *to the operator defined via the kernel*

$$\gamma_\Psi(x, y) = N\int_{(\mathbb{R}^d)^{N-1}} \Psi(x, x_2, ..., x_N)\overline{\Psi(y, x_2, ..., x_N)}\mathrm{d}x_2...\mathrm{d}x_N.$$

If $\Psi \in \mathcal{F}(\mathscr{H})$ does not have a fixed particle number, then it is also important to know $\langle \Psi, a(f)a(g)\Psi\rangle$ and $\langle \Psi, a^*(f)a^*(g)\Psi\rangle$. This gives rise to an operator $\alpha_\Psi : \mathscr{H}^* \to \mathscr{H}$.

Definition. *Let* $\mathscr{H}$ *be a Hilbert space and let* $\mathscr{H}^*$ *be its dual (i.e. the space of all continuous linear functionals from* $\mathscr{H}$ *to* $\mathbb{C}$*). Define the mapping* $J : \mathscr{H} \to \mathscr{H}^*$ *by*

$$J(f)(g) = \langle f, g\rangle, \quad \forall f, g \in \mathscr{H}.$$

Note that J *is anti-linear. The adjoint* $J^* : \mathscr{H}^* \to \mathscr{H}$ *is an anti-linear map defined by*

$$\langle J^*u, v\rangle_{\mathscr{H}} = \langle Jv, u\rangle_{\mathscr{H}^*} = \overline{\langle u, Jv\rangle_{\mathscr{H}^*}}, \quad \forall u \in \mathscr{H}^*, v \in \mathscr{H}.$$

By Riesz representation Theorem, J *is an anti-unitary, namely*

$$J^*J = \mathbb{1}_{\mathscr{H}}, \quad JJ^* = \mathbb{1}_{\mathscr{H}^*}.$$

In particular,

$$\langle Ju, Jv\rangle_{\mathscr{H}^*} = \langle v, u\rangle_{\mathscr{H}} = \overline{\langle u, v\rangle_{\mathscr{H}}}, \quad \forall u, v \in \mathscr{H}.$$

Remarks:

- The point here is that we do not identify $\mathscr{H}$ to $\mathscr{H}^*$, but rather think of $\mathscr{H}^* = J\mathscr{H}$ with an anti-unitary J.
- If $\mathscr{H} = L^2(\mathbb{R}^d)$, then we can simply take J as the complex conjugation.

Definition. *Let Ψ be a normalized vector in the bosonic Fock space $\mathcal{F}(\mathscr{H})$ with $\langle \Psi, \mathcal{N}\Psi\rangle < \infty$. We define the* **pairing operator** $\alpha_\Psi : \mathscr{H}^* \to \mathscr{H}$ *by*

$$\langle g, \alpha_\Psi Jf\rangle = \langle \Psi, a(f)a(g)\Psi\rangle, \quad \forall f, g \in \mathscr{H}.$$

Its adjoint $\alpha_\Psi^* : \mathscr{H} \to \mathscr{H}^*$ is defined by

$$\langle \alpha_\Psi^* g, Jf\rangle_{\mathscr{H}^*} = \langle g, \alpha_\Psi Jf\rangle_{\mathscr{H}} = \langle \Psi, a(f)a(g)\Psi\rangle, \quad \forall f, g \in \mathscr{H}.$$

Note that $\alpha_\Psi^* = J\alpha_\Psi J$.

Remarks:

- The advantage of introducing the anti-linear isomorphism $J : \mathscr{H} \to \mathscr{H}^*$ is that α_Ψ and α_Ψ^* are linear maps.
- The relation $\alpha_\Psi^* = J\alpha_\Psi J$ can be seen from the definition of α_Ψ^* and the CCR:

$$\begin{aligned}\langle \alpha_\Psi^* g, Jf\rangle_{\mathscr{H}^*} &= \langle \Psi, a(f)a(g)\Psi\rangle = \langle \Psi, a(g)a(f)\Psi\rangle \\ &= \langle f, \alpha_\Psi Jg\rangle_{\mathscr{H}} = \langle J\alpha_\Psi Jg, Jf\rangle_{\mathscr{H}^*}, \quad \forall f, g \in \mathscr{H}.\end{aligned}$$

- The relation $\alpha_\Psi^* = J\alpha_\Psi J$ is equivalent to the fact that the kernel $\alpha_\Psi(\cdot,\cdot)$ of α_Ψ is symmetric. We can think of $\mathscr{H} = L^2(\mathbb{R}^d)$ for simplicity, where the kernel $\alpha_\Psi(\cdot,\cdot)$ of α_Ψ is defined as

$$(\alpha_\Psi Jf)(x) = \int \alpha_\Psi(x, y)(Jf)(y)\mathrm{d}y, \quad \forall f \in L^2(\mathbb{R}^d).$$

Then by the definition of α_Ψ, we can write

$$\langle g \otimes f, \alpha_\Psi(\cdot,\cdot)\rangle = \iint \overline{g(x)f(y)}\alpha_\Psi(x, y)\mathrm{d}x\mathrm{d}y = \int \overline{g(x)}(\alpha_\Psi Jf)(x)\mathrm{d}x$$

$$= \langle g, \alpha_\Psi J f\rangle = \langle \Psi, a(f)a(g)\Psi\rangle, \quad \forall f, g \in L^2(\mathbb{R}^d).$$

In particular, since $a(f)a(g) = a(g)a(f)$ by the CCR, we deduce that

$$\langle g \otimes f, \alpha_\Psi(\cdot,\cdot)\rangle = \langle f \otimes g, \alpha_\Psi(\cdot,\cdot)\rangle$$

and hence the kernel $\alpha_\Psi(\cdot,\cdot)$ is symmetric, i.e. an element of $\mathscr{H}^{\otimes_s 2}$.

Definition. *Let Ψ be a normalized vector in the bosonic Fock space $\mathcal{F}(\mathscr{H})$ with $\langle \Psi, \mathcal{N}\Psi\rangle < \infty$. We define the* **generalized one-body density matrix** Γ_Ψ *as an operator on $\mathscr{H} \oplus \mathscr{H}^*$ by the block matrix form*

$$\Gamma_\Psi := \begin{pmatrix} \gamma_\Psi & \alpha_\Psi \\ \alpha_\Psi^* & 1 + J\gamma_\Psi J^* \end{pmatrix} = \begin{pmatrix} \gamma_\Psi & \alpha_\Psi \\ J\alpha_\Psi J & 1 + J\gamma_\Psi J^* \end{pmatrix}$$

Theorem. *Let Ψ be a normalized vector in the bosonic Fock space $\mathcal{F}(\mathscr{H})$ with $\langle \Psi, \mathcal{N}\Psi\rangle < \infty$. Then $\Gamma_\Psi \geq 0$ on $\mathscr{H} \oplus \mathscr{H}^*$. This is equivalently to the operator inequality*

$$\gamma_\Psi \geq J^* \alpha_\Psi^* (1 + \gamma_\Psi)^{-1} \alpha_\Psi J \text{ on } \mathscr{H}.$$

Consequently,

$$\mathrm{Tr}(\alpha_\Psi \alpha_\Psi^*) \leq (1 + \|\gamma_\Psi\|_{\mathrm{op}})\,\mathrm{Tr}(\gamma_\Psi) < \infty.$$

Proof. **Step 1.** By the definitions of γ_Ψ, α_Ψ and the CCR we can write

$$\langle f \oplus Jg, \Gamma_\Psi f \oplus Jg\rangle_{\mathscr{H}\oplus\mathscr{H}^*} = \left\langle \begin{pmatrix} f \\ Jg \end{pmatrix}, \begin{pmatrix} \gamma_\Psi & \alpha_\Psi \\ J\alpha_\Psi J & 1 + J\gamma_\Psi J^* \end{pmatrix} \begin{pmatrix} f \\ Jg \end{pmatrix} \right\rangle_{\mathscr{H}\oplus\mathscr{H}^*}$$

$$= \langle f, \gamma_\Psi f\rangle_{\mathscr{H}} + \langle f, \alpha_\Psi Jg\rangle_{\mathscr{H}} + \langle Jg, J\alpha_\Psi J f\rangle_{\mathscr{H}^*} + \langle Jg, (1 + J\gamma_\Psi J^*)Jg\rangle_{\mathscr{H}^*}$$

$$= \langle f, \gamma_\Psi f\rangle_{\mathscr{H}} + \langle f, \alpha_\Psi Jg\rangle_{\mathscr{H}} + \overline{\langle g, \alpha_\Psi J f\rangle_{\mathscr{H}}} + \|g\|^2_{\mathscr{H}} + \langle g, \gamma_\Psi g\rangle_{\mathscr{H}}$$

$$= \langle \Psi, a^*(f)a(f)\Psi\rangle + \langle \Psi, a(g)a(f)\Psi\rangle + \langle \Psi, a^*(f)a^*(g)\Psi\rangle + \|g\|^2_{\mathscr{H}} + \langle \Psi, a^*(g)a(g)\Psi\rangle$$

$$= \left\langle \Psi, \Big(a^*(f) + a(g)\Big)\Big(a^*(g) + a(f)\Big)\Psi \right\rangle = \left\| \Big(a^*(g) + a(f)\Big)\Psi \right\|^2_{\mathcal{F}} \geq 0$$

for all $f, g \in \mathscr{H}$. Thus $\Gamma_\Psi \geq 0$.

Step 2. From the above proof, we can also see that $\Gamma_\Psi \geq 0$ is equivalent to

$$\langle f, \gamma_\Psi f\rangle + \langle g, (1+\gamma_\Psi)g\rangle \geq 2\Re\langle g, \alpha_\Psi J f\rangle, \quad \forall f, g \in \mathscr{H}.$$

By replacing $f \mapsto \lambda f$ and optimizing over $\lambda \in \mathbb{C}$, we get

$$\langle f, \gamma_\Psi f\rangle \langle g, (1+\gamma_\Psi)g\rangle \geq |\langle g, \alpha_\Psi J f\rangle|^2, \quad \forall f, g \in \mathscr{H}.$$

Replacing g by $(1+\gamma_\Psi)^{-1}g$ we get the equivalent formula

$$\langle f, \gamma_\Psi f\rangle \langle g, (1+\gamma_\Psi)^{-1}g\rangle \geq |\langle g, (1+\gamma_\Psi)^{-1}\alpha_\Psi J f\rangle|^2, \quad \forall f, g \in \mathscr{H}.$$

Then choosing $g = \alpha_\Psi J f$ we find that

$$\langle f, \gamma_\Psi f\rangle \geq \langle \alpha_\Psi J f, (1+\gamma_\Psi)^{-1}\alpha_\Psi J f\rangle = \langle f, J^*\alpha_\Psi^*(1+\gamma_\Psi)^{-1}\alpha_\Psi J f\rangle, \quad \forall f \in \mathscr{H}.$$

Thus we obtain the operator inequality

$$\gamma_\Psi \geq J^*\alpha_\Psi^*(1+\gamma_\Psi)^{-1}\alpha_\Psi J \text{ on } \mathscr{H}.$$

Step 3. Reversely, let us start from the operator inequality

$$\gamma_\Psi \geq J^*\alpha_\Psi^*(1+\gamma_\Psi)^{-1}\alpha_\Psi J \text{ on } \mathscr{H}.$$

Then

$$\langle f, \gamma_\Psi f\rangle \geq \langle \alpha_\Psi J f, (1+\gamma_\Psi)^{-1}\alpha_\Psi J f\rangle = \|(1+\gamma_\Psi)^{-1/2}\alpha_\Psi J f\|^2, \quad \forall f \in \mathscr{H}.$$

Therefore, by the Cauchy-Schwarz inequality we can bound

$$\begin{aligned}&\langle f, \gamma_\Psi f\rangle \langle g, (1+\gamma_\Psi)g\rangle \geq \|(1+\gamma_\Psi)^{-1/2}\alpha_\Psi J f\|^2 \|(1+\gamma_\Psi)^{-1/2}g\|^2 \\ &\geq |\langle (1+\gamma_\Psi)^{-1/2}g, (1+\gamma_\Psi)^{-1/2}\alpha_\Psi J f\rangle|^2 = |\langle g, (1+\gamma_\Psi)^{-1}\alpha_\Psi J f\rangle|^2, \quad \forall f, g \in \mathscr{H}\end{aligned}$$

which is equivalent to $\Gamma_\Psi \geq 0$. *q.e.d.*

The above Theorem gives rise to a **natural question**: given an operator on $\mathscr{H} \oplus \mathscr{H}^*$ of the block matrix form

$$\Gamma := \begin{pmatrix} \gamma & \alpha \\ \alpha^* & 1 + J\gamma J^* \end{pmatrix}$$

satisfying that $\Gamma \geq 0$ and $\alpha^* = J\alpha J$, $\operatorname{Tr}\gamma < \infty$. Then is Γ the generalized one-body density matrix of a state on the bosonic Fock space $\mathcal{F}(\mathscr{H})$? The answer is **yes**, provided that we extend the consideration to **mixed states**.

Definition. *Let G be a* **mixed state** *on the bosonic Fock space $\mathcal{F} = \mathcal{F}(\mathscr{H})$, namely $G \geq 0$ on $\mathcal{F}$ and $\operatorname{Tr}_{\mathcal{F}} G = 1$, with $\operatorname{Tr}_{\mathcal{F}}(\mathcal{N}G) < \infty$. We define the* **generalized one-body density matrix** *of G as an operator on $\mathscr{H} \oplus \mathscr{H}^*$ of the block matrix form*

$$\Gamma_G := \begin{pmatrix} \gamma_G & \alpha_G \\ \alpha_G^* & 1 + J\gamma_G J^* \end{pmatrix}$$

where $\gamma_G : \mathscr{H} \to \mathscr{H}$ and $\alpha_G : \mathscr{H}^* \to \mathscr{H}$ are linear maps defined by

$$\langle g, \gamma_G f\rangle_{\mathscr{H}} = \operatorname{Tr}(a^*(f)a(g)G), \quad \langle g, \alpha_G J f\rangle_{\mathscr{H}} = \operatorname{Tr}(a(f)a(g)G), \quad \forall f, g \in \mathscr{H}.$$

In case $G = |\Psi\rangle\langle\Psi|$ for a normalized vector $\Psi \in \mathcal{F}(\mathscr{H})$, we say that G is a pure state. All of the results discussed above for pure states extend to mixed states, in particular

$$\Gamma_G \geq 0, \quad \alpha_G^* = J\alpha_G J, \quad \operatorname{Tr}\gamma_G = \operatorname{Tr}_{\mathcal{F}}(\mathcal{N}G) < \infty.$$

We will prove that any such a block-matrix operators on $\mathscr{H} \oplus \mathscr{H}^*$ is a one-body density matrix of a mixed state. Moreover, the mixed state can be chosen in a special class called **quasi-free states**.

5.4 Coherent/Gaussian/Quasi-free states

In this section we introduce some special states on Fock space which are relevant to the analysis of the Bose-Einstein condensation and fluctuations around the condensate.
First, we consider **coherent states** of the form

$$e^{-\|f\|^2/2} e^{a^*(f)}\Omega = e^{-\|f\|^2/2} \bigoplus_{n\geq 0} \frac{f^{\otimes n}}{\sqrt{n!}}.$$

This is the analogue of Hartree states $u^{\otimes N}$ on Fock space. Similar to Hartree states, coherent states can be used to describe the Bose-Einstein condensate.

Definition. *Let $\mathscr{H}$ be a one-body Hilbert space. For every $f \in \mathscr{H}$ (not necessarily normalized), we define the* **Weyl operator** $W(f)$ *as a unitary operator on the bosonic Fock space $\mathcal{F} = \mathcal{F}(\mathscr{H})$ by*

$$W(f) = \exp(a^*(f) - a(f)).$$

Then $W(f)\Omega$ is called **a coherent state**.

Theorem. *For every $f \in \mathscr{H}$, the Weyl operator $W(f)$ on $\mathcal{F}(\mathscr{H})$ satisfies*

$$W^*(f)a(g)W(f) = a(g) + \langle g, f\rangle, \quad W^*(f)a^*(g)W(f) = a^*(g) + \langle f, g\rangle, \quad \forall g \in \mathscr{H}.$$

Proof. We will use a "Grönwall argument". In general, if we have two operator A and B, then

$$\frac{d}{dt}(e^{-tA}Be^{tA}) = e^{-tA}(-AB + BA)e^{tA} = e^{-tA}[B, A]e^{tA}.$$

Therefore, integrating over $t \in [0, 1]$ we find that

$$e^{-A}Be^{A} - B = \int_0^1 e^{-tA}[B, A]e^{tA}\mathrm{d}t.$$

Now we apply this identity to $A = a^*(f) - a(f)$ and $B = a(g)$. By the CCR,

$$[B, A] = [a(g), a^*(f) - a(f)] = \langle g, f\rangle$$

and hence

$$e^{-tA}[B, A]e^{tA} = \langle g, f\rangle e^{-tA}e^{tA} = \langle g, f\rangle.$$

Therefore,

$$W^*(f)a(g)W(f) - a(g) = e^{-A}Be^{A} - B = \int_0^1 e^{-tA}[B, A]e^{tA}\mathrm{d}t = \langle g, f\rangle.$$

By the adjointness, it is equivalent to

$$W^*(f)a^*(g)W(f) - a^*(g) = \overline{\langle g, f\rangle} = \langle f, g\rangle.$$

q.e.d.

Exercise. *Let $f \in \mathscr{H}$ and consider Weyl operator $W(f)$ on $\mathcal{F}(\mathscr{H})$. Prove that the corresponding coherent state is*

$$\Psi := W(f)\Omega = e^{-\|f\|^2/2} e^{a^*(f)}\Omega = e^{-\|f\|^2/2} \bigoplus_{n\geq 0} \frac{f^{\otimes n}}{\sqrt{n!}}.$$

Prove that

$$\langle \Psi, \mathcal{N}\Psi\rangle = \|f\|^2_{\mathscr{H}}.$$

Next, we consider **excited particles** outside of the condensate. We will focus on the **quasi-free states**, where the excited particles come in pairs. The simplest examples of **quasi-free states** are **Gaussian states**

Theorem (Gaussian states)**.** *Let $h > 0$ be self-adjoint on $\mathscr{H}$ such that $\mathrm{Tr}(e^{-h}) < \infty$. Then we have the following properties.*

- *The* **partition function** *is*

$$Z := \mathrm{Tr}\, e^{-\mathrm{d}\Gamma(h)} = \exp\Big(- \mathrm{Tr}(\log(1-e^{-h}))\Big) \in (0,\infty).$$

  Consequently, the **Gaussian state** $G = Z^{-1}e^{-\mathrm{d}\Gamma(h)}$ *is well-defined.*

- *The one-body density matrix of G is*

$$\gamma_G = \frac{1}{e^h - 1}.$$

  This is a non-negative trace class operator on $\mathscr{H}$, namely $\mathrm{Tr}(\mathcal{N}G) < \infty$.

- *The Gaussian state G satisfies* **Wick's Theorem**, *namely*

$$\mathrm{Tr}(a_1^{\#}...a_{2m-1}^{\#}G) = 0, \quad \forall m \geq 1$$

  and

$$\mathrm{Tr}(a_1^{\#}...a_{2m}^{\#}G) = \sum_{\sigma\in P_{2m}} \mathrm{Tr}(a^{\#}_{\sigma(1)}a^{\#}_{\sigma(2)}G)... \mathrm{Tr}(a^{\#}_{\sigma(2m-1)}a^{\#}_{\sigma(2m)}G), \quad \forall m \geq 1.$$

Here $a_n^\#$ is either $a(f_n)$ or $a^*(f_n)$ with arbitrary vectors $(f_1, f_2, ...) \subset \mathscr{H}$. The **set of pairings** *P_{2m} is*

$$P_{2m} = \{\sigma \in S_{2m} \mid \sigma(2j-1) < \sigma(2j+1), j = 1, \dots, m-1, \\ \sigma(2j-1) < \sigma(2j),\ j = 1, \dots, m\}.$$

Remark: Wick's theorem is used extensively in **quantum field theory**, especially in connection to **Feynman diagrams**. As an example, Wick's theorem with order 4 gives

$$\mathrm{Tr}(a_1^* a_2^* a_3 a_4 G) = \mathrm{Tr}(a_1^* a_2^* G)\,\mathrm{Tr}(a_3 a_4 G) + \mathrm{Tr}(a_1^* a_3 G)\,\mathrm{Tr}(a_2^* a_4 G) + \mathrm{Tr}(a_1^* a_4 G)\,\mathrm{Tr}(a_2^* a_3 G)$$

with $a_i = a(f_i)$ for arbitrary vectors $\{f_i\} \subset \mathscr{H}$. In case G is a **normal state**, i.e. $[G, \mathcal{N}] = 0$ (e.g. the Gaussian state), the pairing terms $\mathrm{Tr}(a_1^* a_2^* G)$ and $\mathrm{Tr}(a_3 a_4 G)$ are 0, and we get the simplify formula

$$\mathrm{Tr}(a_1^* a_2^* a_3 a_4 G) = \mathrm{Tr}(a_1^* a_3 G)\,\mathrm{Tr}(a_2^* a_4 G) + \mathrm{Tr}(a_1^* a_4 G)\,\mathrm{Tr}(a_2^* a_3 G).$$

Proof. **Step 1.** The condition $\mathrm{Tr}(e^{-h}) < \infty$ implies that h has compact resolvent. Therefore, we have the spectral decomposition

$$h = \sum_{n \geq 1} \lambda_n |u_n\rangle\langle u_n|$$

with an orthonormal basis $\{u_n\}_{n\geq 1}$ for $\mathscr{H}$ and $0 < \lambda_1 \leq \lambda_2 \leq ...$ with

$$\sum_{n\geq 1} e^{-\lambda_n} = \mathrm{Tr}(e^{-h}) < \infty.$$

Then we can write

$$\mathrm{d}\Gamma(h) = \sum_{n\geq 1} \lambda_n \mathrm{d}\Gamma(|u_n\rangle\langle u_n|) = \sum_{n \geq 1} \lambda_n a_n^* a_n$$

where $a_n = a(u_n)$. Since $a_n^* a_n$ and $a_m^* a_m$ commute, we can decompose

$$e^{-\mathrm{d}\Gamma(h)} = e^{-\sum_n \lambda_n a_n^* a_n} = \prod_n e^{-\lambda_n a_n^* a_n}.$$

Next, recall that the bosonic Fock space $\mathcal{F}(\mathscr{H})$ has an orthonormal basis

$$|n_1, n_2, ...\rangle := (n_1! n_2! ...)^{-1/2} (a_1^*)^{n_1} (a_2^*)^{n_2} ... \Omega.$$

Here $n_1, n_2, ... \in \{0, 1, 2, ...\}$ and there are only finitely many $n_k > 0$. Let us compute

$$e^{-\mathrm{d}\Gamma(h)}|n_1, n_2, ...\rangle = \prod_i e^{-\lambda_i a_i^* a_i}|n_1, n_2, ...\rangle.$$

For every $i = 1, 2, ...$ we have

$$\frac{d}{d\lambda}e^{-\lambda a_i^* a_i}|n_1, n_2, ...\rangle = -e^{-\lambda a_i^* a_i}(a_i^* a_i)|n_1, n_2, ...\rangle = -n_i e^{-\lambda a_i^* a_i}|n_1, n_2, ...\rangle$$

for all $\lambda \geq 0$. Here we used the fact that $|n_1, n_2, ...\rangle$ has exactly n_i particles in the mode u_i. Integrating over $\lambda \in [0, \lambda_i]$ gives

$$e^{-\lambda_i a_i^* a_i}|n_1, n_2, ...\rangle = e^{-\lambda_i n_i}|n_1, n_2, ...\rangle$$

for all $i = 1, 2, ...$ (The latter equality can be also deduced from the Spectral Theorem and the fact that $|n_1, n_2, ...\rangle$ is an eigenfunction of $a_i^* a_i$ with eigenvalue n_i). Thus

$$e^{-\mathrm{d}\Gamma(h)}|n_1, n_2, ...\rangle = \prod_i e^{-\lambda_i a_i^* a_i}|n_1, n_2, ...\rangle = \prod_i e^{-\lambda_i n_i}|n_1, n_2, ...\rangle.$$

This means that all eigenvalues of $e^{-\mathrm{d}\Gamma(h)}$ are $\prod_{i\geq 1} e^{-\lambda_i n_i}$, and hence

$$Z = \operatorname{Tr} e^{-\mathrm{d}\Gamma(h)} = \sum_{n_i=0,1,2,...} \prod_{i\geq 1} e^{-\lambda_i n_i} = \prod_{i\geq 1}\Big[\sum_{n=0,1,2,...} e^{-\lambda_i n}\Big] = \prod_{i\geq 1}\frac{1}{1-e^{-\lambda_i}}.$$

The result can be rewritten in a "fancy way"

$$-\log Z = \sum_{i\geq 1}\log(1-e^{-\lambda_i}) = \operatorname{Tr}(\log(1-e^{-h}))$$

which is equivalent to $Z = \exp(-\operatorname{Tr}(\log(1-e^{-h})))$. To prove that Z is finite, we need to check

$$\prod_{i\geq 1}(1-e^{-\lambda_i}) > 0,$$

but this follows from the assumption $\sum_{i\geq 1} e^{-\lambda_i} = \operatorname{Tr} e^{-h} < \infty$.

Exercise. *Let $\{s_i\}_{i\geq 1} \subset (0,1)$. Prove that the following two statements are equivalent.*

1. $\sum_{i\geq 1} s_i < \infty$.

2. $\prod_{i\geq 1}(1-s_i) > 0$.

Step 2. Now we compute the one-body density matrix γ_G. Since $\{u_n\}_{n\geq 1}$ is an orthonormal basis for $\mathscr{H}$, it suffices to prove that

$$\langle u_m, \gamma_G u_\ell\rangle = \Big\langle u_m, (e^h-1)^{-1}u_\ell\Big\rangle = \delta_{m=\ell}(e^{\lambda_\ell}-1)^{-1}, \quad \forall m, \ell \geq 1.$$

We compute the left side using the definition of γ_G and the fact that $|n_1, n_2, ...\rangle$ are eigenfunctions of $e^{-\mathrm{d}\Gamma(h)}$ with eigenvalues $\prod_{i\geq 1} e^{-\lambda_i n_i}$. This gives

$$\begin{aligned}
&\langle u_m, \gamma_G u_\ell\rangle = \mathrm{Tr}(a_\ell^* a_m G) = Z^{-1}\,\mathrm{Tr}\left(a_\ell^* a_m e^{-\mathrm{d}\Gamma(h)}\right) \\
&= Z^{-1}\sum_{n_j=0,1,...}\langle n_1, n_2, ...|a_\ell^* a_m e^{-\mathrm{d}\Gamma(h)}|n_1, n_2, ...\rangle \\
&= Z^{-1}\sum_{n_j=0,1,...}\prod_{i\geq 1} e^{-\lambda_i n_i}\langle n_1, n_2, ...|a_\ell^* a_m|n_1, n_2, ...\rangle \\
&= Z^{-1}\sum_{n_j=0,1,...}\prod_{i\geq 1} e^{-\lambda_i n_i} n_\ell \delta_{m=\ell}.
\end{aligned}$$

Using

$$e^{-\lambda_\ell n_\ell} n_\ell = -\frac{d}{d\lambda_\ell} e^{-\lambda_\ell n_\ell}$$

we can simplify

$$\begin{aligned}
&\langle u_m, \gamma_G u_\ell\rangle = \delta_{m=\ell} Z^{-1}\sum_{n_j=0,1,...}\Big(-\frac{d}{d\lambda_\ell}\Big)\prod_{i\geq 1} e^{-\lambda_i n_i} \\
&= \delta_{m=\ell} Z^{-1}\Big(-\frac{d}{d\lambda_\ell}\Big)(Z) = \delta_{m=\ell}(1-e^{-\lambda_\ell})\Big(-\frac{d}{d\lambda_\ell}\Big)\Big[\frac{1}{1-e^{-\lambda_\ell}}\Big] \\
&= \delta_{m=\ell}\frac{e^{-\lambda_\ell}}{1-e^{-\lambda_\ell}} = \delta_{m=\ell}\frac{1}{e^{\lambda_\ell}-1}.
\end{aligned}$$

Thus we conclude that $\gamma_G = (e^h-1)^{-1}$. The fact that $\mathrm{Tr}\,\gamma_G < \infty$ follows from the assumption $\mathrm{Tr}\, e^{-h} < \infty$ (**why?**).

Step 3. Finally, we prove Wick's Theorem. We denote by c_i either a_j or a_j^* (the indexes i and j may be different). Our aim is to show that

$$\begin{aligned}
\mathrm{Tr}[c_1c_2c_3c_4...c_kG] &= \mathrm{Tr}[c_1c_2G]\,\mathrm{Tr}[c_3c_4...c_kG] \\
&\quad + \mathrm{Tr}[c_1c_3G]\,\mathrm{Tr}[c_2c_4...c_kG] + ... + \mathrm{Tr}[c_1c_kG]\,\mathrm{Tr}[c_2c_3...c_{k-1}G]
\end{aligned}$$

and the result follows immediately by induction. By the same way of computing the partition function and the one-body density matrix, we have

$$\mathrm{Tr}[c_1 c_2 G] = f(c_1)[c_1, c_2]$$

where $[c_1, c_2] = c_1 c_2 - c_2 c_1 \in \{0, -1, 1\}$ and

$$f(c_1) = \begin{cases} (1 - e^{-\lambda_j})^{-1} & \text{if } c_1 = a_j, \\ (1 - e^{\lambda_j})^{-1} & \text{if } c_1 = a_j^*. \end{cases}$$

Thus the desired equality is equivalent to

$$\begin{aligned} \mathrm{Tr}[c_1 c_2 c_3 c_4 ... c_k G] &= f(c_1)[c_1, c_2]\,\mathrm{Tr}[c_3 c_4 ... c_k G] \\ &+ f(c_1)[c_1, c_3]\,\mathrm{Tr}[c_2 c_4 ... c_k G] + ... + f(c_1)[c_1, c_k]\,\mathrm{Tr}[c_2 c_3 ... c_{k-1} G]. \end{aligned}$$

Let us focus on the last equality. From the identity

$$c_1 c_2 c_3 c_4 ... c_k = [c_1, c_2] c_3 c_4 ... c_k + ... + c_2 c_4 ... c_{k-1} [c_1, c_k] + c_2 c_3 c_4 ... c_k c_1$$

we deduce that

$$\begin{aligned} \mathrm{Tr}\left[c_1 c_2 c_3 c_4 ... c_k G\right] &= \mathrm{Tr}\left[[c_1, c_2] c_3 c_4 ... c_k G\right] \\ &+ ... + \mathrm{Tr}\left[c_2 c_4 ... c_{k-1} [c_1, c_k] G\right] + \mathrm{Tr}\left[c_2 c_3 c_4 ... c_k c_1 G\right]. \end{aligned}$$

It is straightforward to see that $c_1 G = e^{\pm\lambda_j} G c_1$ where (+) if $c_1 = a_j^*$ and (-) if $c_1 = a_j$. This implies that

$$\mathrm{Tr}\left[c_2 c_3 c_4 ... c_k c_1 G\right] = e^{\pm\lambda_j} \mathrm{Tr}\left[c_2 c_3 c_4 ... c_k G c_1\right] = e^{\pm\lambda_j} \mathrm{Tr}\left[c_1 c_2 c_3 c_4 ... c_k G\right].$$

From that and the definition of f we conclude that

$$\begin{aligned} \mathrm{Tr}\left[c_1 c_2 c_3 c_4 ... c_k G\right] &= \frac{[c_1, c_2]}{1 - e^{\pm\lambda_j}} \mathrm{Tr}\left[c_3 c_4 ... c_k G\right] \\ &+ \frac{[c_1, c_3]}{1 - e^{\pm\lambda_j}} \mathrm{Tr}\left[c_2 c_4 ... c_k G\right] + ... + \frac{[c_1, c_k]}{1 - e^{\pm\lambda_j}} \mathrm{Tr}\left[c_2 c_4 ... c_{k-1} G\right] \\ &= f(c_1)[c_1, c_2]\,\mathrm{Tr}[c_3 c_4 ... c_k G] \\ &+ f(c_1)[c_1, c_3]\,\mathrm{Tr}[c_2 c_4 ... c_k G] + ... + f(c_1)[c_1, c_k]\,\mathrm{Tr}[c_2 c_3 ... c_{k-1} G]. \end{aligned}$$

This completes the proof of Wick's theorem. *q.e.d.*

Finally we define

Definition. *Let G be a mixed state on a bosonic Fock space $\mathcal{F}(\mathscr{H})$ with $\operatorname{Tr}(G\mathcal{N}) < \infty$. We call G* **a quasi-free state** *if it satisfies* **Wick's Theorem**, *namely*

$$\operatorname{Tr}(a_1^{\#}...a_{2m-1}^{\#}G) = 0, \quad \forall m \geq 1$$

and

$$\operatorname{Tr}(a_1^{\#}...a_{2m}^{\#}G) = \sum_{\sigma \in P_{2m}} \operatorname{Tr}(a_{\sigma(1)}^{\#}a_{\sigma(2)}^{\#}G)... \operatorname{Tr}(a_{\sigma(2m-1)}^{\#}a_{\sigma(2m)}^{\#}G), \quad \forall m \geq 1.$$

Here $a_n^{\#}$ is either $a(f_n)$ or $a^*(f_n)$ with arbitrary vectors $(f_1, f_2, ...) \subset \mathscr{H}$ and P_{2m} is **set of pairings**

$$P_{2m} = \{\sigma \in S_{2m} \mid \sigma(2j-1) < \sigma(2j+1), j = 1, \dots, m-1,$$
$$\sigma(2j-1) < \sigma(2j),\ j = 1, \dots, m\}.$$

- *If a quasi-free state is a pure state $|\Psi\rangle\langle\Psi|$, we call it a* **pure** *quasi-free state.*
- *If a quasi-free state G commutes with the number operator, i.e. $[G, \mathcal{N}] = 0$, we call it a* **normal** *quasi-free state. In this case, the paring operator vanishes $\alpha_G = 0$.*

In principle, any quasi-free state G on $\mathcal{F}(\mathscr{H})$ is determined completely by its generalized one-body density matrix

$$\Gamma_G := \begin{pmatrix} \gamma_G & \alpha_G \\ \alpha_G^* & 1 + J\gamma_G J^* \end{pmatrix}.$$

Moreover, from the general discussion in the previous section we know that $\Gamma_G \geq 0$ on $\mathscr{H} \oplus \mathscr{H}^*$, $\alpha_G^* = J\alpha_G J$ and $\operatorname{Tr} \gamma_G < \infty$. The reverse is also true, namely any block-matrix operator of this form is a

Thus a **natural question** is that given an operator on $\mathscr{H} \oplus \mathscr{H}^*$ of the block matrix form is the generalized one-body density matrix of a quasi-free state.

Theorem 5.1. *Consider a bounded linear operator on* $\mathscr{H} \oplus \mathscr{H}^*$

$$\Gamma := \begin{pmatrix} \gamma & \alpha \\ \alpha^* & 1 + J\gamma J^* \end{pmatrix}.$$

with $\Gamma \geq 0$, $\alpha^* = J\alpha J$, $\operatorname{Tr}\gamma < \infty$. *Then there exists* **a unique (mixed) quasi-free state** G *on the bosonic Fock space* $\mathcal{F}(\mathscr{H})$ *such that* $\Gamma = \Gamma_G$*, the generalized one-body density matrix of* G. □

The proof of this theorem requires to use **Bogoliubov transformations** which will be introduced in the next chapter.

Exercise. *Let* $\mathcal{N}$ *be the number operator on a bosonic Fock space* $\mathcal{F}(\mathscr{H})$*. Let* $N \in \mathbb{N}$ *be a large parameter.*

1. *Prove that*

$$N^2 = \inf\Big\{ \operatorname{Tr}(\mathcal{N}^2 G) \,|\; G \text{ a mixed state on } \mathcal{F}(\mathscr{H}) \text{ satisfying } \operatorname{Tr}(\mathcal{N}G) = N \Big\}.$$

2. *Let* Ψ *be an arrbitrary coherent state satisfying* $\langle \Psi, \mathcal{N}\Psi\rangle = N$*. Prove that*

$$\langle \Psi, \mathcal{N}^2 \Psi\rangle = N^2 + N.$$

3. *Consider the variational problem*

$$E_N = \inf\Big\{ \operatorname{Tr}(\mathcal{N}^2 G) \,|\, G = W^*(f) K W(f), f \in \mathscr{H} \text{ and } \\ K \text{ a (mixed) quasi-free state such that } \operatorname{Tr}(\mathcal{N}G) = N \Big\}.$$

Prove that $E_N = N^2 + O(N^{2/3})$.

Hint: You can write $\mathcal{N}(\mathcal{N}-1) = \sum_{m,n\geq 1} a_m^* a_n^* a_m a_n$ *with* $a_n = a(u_n)$ *for an orthonormal basis* $\{u_n\}$ *for* $\mathscr{H}$*. You can use the result on the correspondence between* G *and* Γ_G.

Chapter 6

Bogoliubov theory

6.1 Bogoliubov heuristic argument

In 1947, Bogoliubov suggested an approximation method to study the low lying spectrum of interacting Bose gases. Recall that the typical N-body Hamiltonian with pair interactions

$$H_N = \sum_{i=1}^{N} h_i + \sum_{1 \le i < j \le N} W_{ij}$$

on $\mathscr{H}^{\otimes_s N}$ can be extended to be an operator on the bosonic Fock space $\mathcal{F}(\mathscr{H})$ as

$$\mathbb{H} = \sum_{m,n \ge 0} h_{mn} a_m^* a_n + \frac{1}{2} \sum_{m,n,p,q \ge 0} W_{mnpq} a_m^* a_n^* a_p a_q$$

where $a_n = a(u_n)$ with an orthonormal basis $\{u_n\}_{n \ge 0}$ for $\mathscr{H}$ and

$$h_{mn} = \langle u_m, h u_n \rangle_{\mathscr{H}}\,, \quad W_{mnpq} = \langle u_m \otimes u_n, W u_p \otimes u_q \rangle_{\mathscr{H}^{\otimes 2}}\,.$$

Bogoliubov suggested that after factoring out the contribution of the Bose-Einstein condensate described by u_0, then the contribution from **excited particles** (orthogonal to u_0) can be effectively described by a **quadratic Hamiltonian** on Fock space $\mathcal{F}(\{u_0\}^{\perp})$.

Definition (Bogoliubov's approximation method).

- **Step 1 (Ignoring higher order terms)** *In the second quantization form*

$$\mathbb{H} = \sum_{m,n\geq 0} h_{mn} a_m^* a_n + \frac{1}{2} \sum_{m,n,p,q\geq 0} W_{mnpq} a_m^* a_n^* a_p a_q$$

we ignore all terms with 3 or 4 operators $a_{n\neq 0}^\#$ *(*$a_n^\#$ *is either* a_n^* *or* a_n*).*

- **Step 2 (c-number substitution)** *Replacing the operators* $a_0^\#$ *by a scalar number* $\sqrt{N_0}$ *with* $N_0 > 0$*.*

- **Step 3 (Cancelation of linear terms)** *The linear terms containing only one* $a_{n\neq 0}^\#$ *are cancelled by the property of* u_0

$$\widetilde{h} u_0 \approx 0, \quad \widetilde{h} := h + N_0(W * |u_0|^2) - \mu.$$

- **Step 4 (Quadratic approximation)** *We get* $\mathbb{H} \approx E_0 + \mathbb{H}_{\mathrm{Bog}}$ *with* $E_0 \in \mathbb{R}$ *and*

$$\mathbb{H}_{\mathrm{Bog}} = \sum_{m,n\geq 1} (\widetilde{h}_{mn} + N_0 W_{m00n}) a_m^* a_n + \frac{1}{2} \sum_{m,n\geq 1} \Big(N_0 W_{mn00} a_m^* a_n^* + h.c. \Big).$$

Here we write $X + h.c.$ *for* $X + X^*$*. This* **quadratic Hamiltonian** *can be* **exactly diagonalized***, leading to an effective description for the spectrum of* $\mathbb{H}$*.*

Explanation:

- Motivation of **Step 1 (Ignoring higher order terms)**: most of particles occupy the condensate described by u_0, and there are very few particles in the excited modes $\{u_n\}_{n\neq 0}$. Therefore, the contribution from $a_{n\neq 0}^\#$ is much smaller than $a_0^\#$, allowing us to ignore terms higher than quadratic in $a_{n\neq 0}^\#$.

- Motivation of **Step 2 (c-number substitution)**: the condensation on the mode u_0 implies $\langle a_0^* a_0 \rangle = N_0 \gg 1$ while $[a_0, a_0^*] = 1$. Hence we can think of a_0 and a_0^* as they commuted. The most natural candidate for the c-number substitution is thus $\sqrt{N_0}$.

  Technically, since the term $a_0^* a_0^* a_0 a_0$ is quite large, we should rewrite

$$a_0^* a_0^* a_0 a_0 = a_0^* a_0 (a_0^* a_0 - 1)$$

before applying the c-number substitution. The first two steps result in

$$\mathbb{H} \approx N_0 h_{00} + \frac{N_0(N_0-1)}{2} W_{0000} + \sqrt{N_0} \sum_{m\geq 1} \Big[(h_{0m} + N_0 W_{000m}) a_m + h.c.\Big]$$
$$+ \sum_{m,n\geq 1} (h_{mn} + N_0 W_{m0n0} + N_0 W_{m00n}) a_m^* a_n + \frac{1}{2} \sum_{m,n\geq 1} \Big(N_0 W_{mn00} a_m^* a_n^* + h.c.\Big).$$

- **Step 3 (Cancelation of linear terms)** essentially follows from Hartree equation. More precisely, from the leading order behavior of u_0, we can expect that

$$\widetilde{h} u_0 \approx 0, \quad \widetilde{h} := h + N_0(W * |u_0|^2) - \mu.$$

Consequently, for every $m \neq 0$,

$$h_{0m} + N_0 W_{000m} = \Big\langle u_m, \Big(h + N_0(W * |u_0|^2)\Big) u_0 \Big\rangle \approx \Big\langle u_m, \mu u_0 \Big\rangle = 0.$$

- Finally, given that the total particle number is N, we can rewrite $N_0 = N - N_+$ where

$$N_+ = \langle \sum_{n\geq 1} a_n^* a_n \rangle.$$

Therefore, when think of the mean-field situation $W_{0000} \sim 1/N$ we obtain

$$N_0 h_{00} + \frac{N_0(N_0-1)}{2} W_{0000} = (N - N_+) h_{00} + \frac{(N-N_+)^2}{2} W_{0000} - \frac{N_0}{2} W_{0000}$$
$$= N h_{00} + \frac{N^2}{2} W_{0000} - N_+(h_{00} + N W_{0000}) - \frac{N_0}{2} W_{0000} + \frac{\mathcal{N}_+^2}{2} W_{0000}$$
$$\approx N h_{00} + \frac{N^2}{2} W_{0000} - (h_{00} + N_0 W_{0000}) N_+ - \frac{N}{2} W_{0000}$$
$$= N h_{00} + \frac{N(N-1)}{2} W_{0000} - \mu N_+ \approx E_0 + \frac{N(N-1)}{2} W_{0000} - \mu \sum_{n\geq 1} a_n^* a_n$$

with

$$E_0 = N h_{00} + \frac{N(N-1)}{2} W_{0000} = N e_{\mathrm{H}}.$$

Thus we end up with **Step 4 (Quadratic approximation)**

$$\mathbb{H} \approx N e_{\mathrm{H}} - \mu \sum_{n\geq 1} a_n^* a_n$$

$$+ \sum_{m,n\geq 1} (h_{mn} + N_0 W_{m0n0} + N_0 W_{m00n}) a_m^* a_n + \frac{1}{2} \sum_{m,n\geq 1} \Big(N_0 W_{mn00} a_m^* a_n^* + h.c. \Big)$$

$$= N e_{\rm H} + \sum_{m,n\geq 1} (\widetilde{h}_{mn} + N_0 W_{m00n}) a_m^* a_n + \frac{1}{2} \sum_{m,n\geq 1} \Big(N_0 W_{mn00} a_m^* a_n^* + h.c. \Big).$$

- The quadratic Hamiltonian

$$\mathbb{H}_{\rm Bog} = \sum_{m,n\geq 1} (\widetilde{h}_{mn} + N_0 W_{m00n}) a_m^* a_n + \frac{1}{2} \sum_{m,n\geq 1} \Big(N_0 W_{mn00} a_m^* a_n^* + h.c. \Big).$$

acts on the **excited Fock space** $\mathcal{F}(\{u_0\}^\perp)$. In principle, it can be rewritten as a **non-interacting Hamiltonian** up to a unitary transformation $\mathbb{U}$ on $\mathcal{F}$ (called **a Bogoliubov transformation**), namely

$$\mathbb{U}^* \mathbb{H}_{\rm Bog} \mathbb{U} = e_{\rm Bog} + {\rm d}\Gamma(\xi)$$

with $e_{\rm Bog}$ the ground state energy of $\mathbb{H}_{\rm Bog}$ and $\xi \geq 0$ a one-body self-adjoint operator on $\mathscr{H}_+ = \{u_0\}^\perp$. Thus in summary,

$$\mathbb{H} \approx N e_{\rm H} + \mathbb{H}_{\rm Bog} = N e_{\rm H} + e_{\rm Bog} + \mathbb{U} {\rm d}\Gamma(\xi) \mathbb{U}^*.$$

The spectrum of the non-interacting Hamiltonian is easy to understand

$$\sigma({\rm d}\Gamma(\xi)) = \Big\{ \sum_k n_k e_k \,|\, e_k \in \sigma(\xi), n_k = 0, 1, 2, ... \Big\}$$

leading to an effective description for the spectrum of $\mathbb{H}$. More precisely, the **low lying eigenvalues** of $\mathbb{H}$ are of the form

$$N e_{\rm H} + e_{\rm Bog} + \sum_k n_k e_k$$

where $e_k \in \sigma(\xi)$ called **elementary excitations** and $n_k = 0, 1, 2, ...$ Here we have finite sum, namely there are only finitely many $n_k > 0$. In particular, the lowest eigenvalue is

$$\inf \sigma(\mathbb{H}) \approx N e_{\rm H} + e_{\rm Bog}$$

and the ground state is approximately $\mathbb{U}\Omega$ (after removing the condensation). We will see later that when $\mathbb{U}$ is a Bogoliubov transformation, then $\mathbb{U}\Omega$ is a **quasi-free state**.

Remark: **Bogoliubov's approximation is a quantized version of Taylor's expansion** of the Hartree functional. Recall that if x_0 is a local minimizer of a smooth function $f:\mathbb{R}\to\mathbb{R}$ then near x_0 we have Taylor's expansion

$$\begin{aligned} f(x) &= f(x_0) + f'(x_0)(x-x_0) + \frac{1}{2}f''(x_0)(x-x_0)^2 + o(|x-x_0|^2) \\ &= f(x_0) + \frac{1}{2}f''(x_0)(x-x_0)^2 + o(|x-x_0|^2). \end{aligned}$$

Here the first derivative $f'(x_0)=0$ because the minimizing property of x_0. Similarly, near the minimizer u_0 of the Hartree functional (we think of the case $\mathscr{H}=L^2(\mathbb{R}^d)$)

$$\mathcal{E}_{\rm H}(u) = \langle u, hu\rangle + \iint (N-1)W(x-y)|u(x)|^2|u(y)|^2 {\rm d}x{\rm d}y$$

under the constraint $\|u\|=1$ we can write for $v\in\{u_0\}^\perp$

$$\mathcal{E}_{\rm H}\left(\frac{u_0+v}{(1+\|v\|^2)^{1/2}}\right) = \mathcal{E}_{\rm H}(u_0) + \frac{1}{2}{\rm Hess}\,\mathcal{E}_{\rm H}(u_0)(v,v) + o\big(\langle v,(h+C)v\rangle\big).$$

The Hessian operator is

$$\begin{aligned} &\frac{1}{2}{\rm Hess}\,\mathcal{E}_{\rm H}(u_0)(v,v) \\ &= \langle v, \widetilde{h}v\rangle + \frac{1}{2}\iint w(x-y)\Big(\overline{v(x)}u_0(x)\overline{u_0(y)}v(y) + v(x)\overline{u_0(x)}u_0(y)\overline{v(y)} \\ &\qquad + \overline{v(x)}u_0(x)u_0(y)\overline{v(y)} + v(x)\overline{u_0(x)u_0(y)}v(y)\Big){\rm d}x\,{\rm d}y \\ &= \frac{1}{2}\left\langle \begin{pmatrix} v \\ \overline{v}\end{pmatrix} \begin{pmatrix} \widetilde{h}+K_1 & K_2 \\ K_2^* & \overline{\widetilde{h}}+\overline{K_1}\end{pmatrix} \begin{pmatrix} v \\ \overline{v}\end{pmatrix}\right\rangle \end{aligned}$$

Here we identify $L^2(\mathbb{R}^d)^* = \overline{L^2(\mathbb{R}^d)}$ and K_1, K_2 are operators on $L^2(\mathbb{R}^d)$ with kernels

$$K_1(x,y) = u_0(x)\overline{u_0(y)}(N-1)W(x-y), \quad K_2(x,y) = u_0(x)u_0(y)(N-1)W(x-y).$$

The second quantization form of the Hessian matrix can be obtained by formally replacing $\overline{v(x)}$ by an operator $a^*(x)$ which creates an excited particle at x, and $v(x)$ by an operator $a(x)$ which annihilates it. This gives

$$\mathbb{H}_{\rm Bog} := \iint (\widetilde{h}+K_1)(x,y)a_x^*a_y{\rm d}x{\rm d}y + \frac{1}{2}\iint \Big(K_2(x,y)a^*(x)a^*(y) + \overline{K_2(x,y)}a(x)a(y)\Big){\rm d}x\,{\rm d}y.$$

Here we are working on the excited Fock space $\mathcal{F}(\{u_0\}^\perp)$. This is the same to write

$$\mathbb{H}_{\rm Bog} = \sum_{m,n\geq 1} \langle u_m, (\widetilde{h} + K_1) u_n \rangle a_m^* a_n + \frac{1}{2} \sum_{m,n\geq 1} \Big(\langle u_m \otimes u_n, K_2 \rangle a_m^* a_n^* + h.c. \Big)$$

which coincides to

$$\sum_{m,n\geq 1} (\widetilde{h}_{mn} + N_0 W_{m00n}) a_m^* a_n + \frac{1}{2} \sum_{m,n\geq 1} \Big(N_0 W_{mn00} a_m^* a_n^* + h.c. \Big).$$

up to a small adjustment $N_0 \approx (N-1)$.

6.2 Example for the homogeneous gas

Let us consider the simplest model where we have N bosons in a unit torus $\mathbb{T}^d$ (i.e. $[0,1]^d$ with periodic boundary condition). The particles interacts via an interaction potential $W = (N-1)^{-1} w$ with

$$w(x) = w(-x) = \sum_{k \in 2\pi\mathbb{Z}^d} \widehat{w}(k) e^{ik\cdot x}.$$

We will assume that the interaction potential is of **positive type and smooth**, namely

$$0 \leq \widehat{w} \in \ell^1(2\pi\mathbb{Z}^d).$$

Here we do not put any external potential, and hence the system is **translation-invariant**. The corresponding N-body Hamiltonian reads

$$H_N = \sum_{i=1}^N (-\Delta_{x_i}) + \frac{1}{N-1} w(x_i - x_j)$$

acting on $L^2(\mathbb{T}^d)^{\otimes_s N}$. In this case, the Hartree theory has a unique minimizer (up to a phase)

$$u_0(x) = 1, \quad \forall x \in \mathbb{T}^d.$$

Exercise. *Consider the Hartree functional*

$$\mathcal{E}_{\rm H}(u) = \int_{\mathbb{T}^d} |\nabla u|^2 + \frac{1}{2} \iint_{\mathbb{T}^d \times \mathbb{T}^d} w(x-y) |u(x)|^2 |u(y)|^2 {\rm d}x{\rm d}y.$$

Prove that if $0 \le \widehat{w} \in \ell^1(2\pi\mathbb{Z}^d)$*, then the Hartree energy is*

$$\inf\left\{\mathcal{E}_{\rm H}(u) \,|\, u \in H^1(\mathbb{T}^d), \|u\|_{L^2(\mathbb{T}^d)} = 1\right\} = \frac{1}{2}\widehat{w}(0).$$

Moreover, $u_0 \equiv 1$ *is the unique Hartree minimizer (uniqueness is up to a phase).*

Now we apply Bogoliubov's heursitic argument to this Hamiltonian. We take the orthonormal basis $\{u_k\}$ for $\mathscr{H} = L^2(\mathbb{T}^d)$ with

$$u_k(x) = e^{ik\cdot x}, \quad \forall k \in 2\pi\mathbb{Z}^d.$$

Then we have

$$\widetilde{h} = -\Delta + N_0(W * |u_0|^2) - \mu = -\Delta$$

($u_0 \equiv 1$ is the unique ground state for $\widetilde{h}$) and

$$\begin{aligned}
N_0 W_{m00n} \approx (N-1)W_{m00n} &= \iint_{\mathbb{T}^d\times\mathbb{T}^d} \overline{u_m(x)u_0(y)}w(x-y)u_0(x)u_n(y)\mathrm{d}x\mathrm{d}y \\
&= \iint_{\mathbb{T}^d\times\mathbb{T}^d} e^{-im\cdot x}\sum_{k\in 2\pi\mathbb{Z}^d}\widehat{w}(k)e^{ik\cdot(x-y)}e^{in\cdot y}\mathrm{d}x\mathrm{d}y \\
&= \sum_{k\in 2\pi\mathbb{Z}^d}\widehat{w}(k)\iint_{\mathbb{T}^d\times\mathbb{T}^d} e^{i(k-m)\cdot x}e^{i(n-k)\cdot y}\mathrm{d}x\mathrm{d}y \\
&= \sum_{k\in 2\pi\mathbb{Z}^d}\widehat{w}(k)\delta_{m=k}\delta_{n=k} \\
&= \delta_{m=n}\widehat{w}(n), \\
N_0 W_{mn00} \approx (N-1)W_{mn00} &= \iint_{\mathbb{T}^d\times\mathbb{T}^d} \overline{u_m(x)u_n(y)}w(x-y)u_0(x)u_0(y)\mathrm{d}x\mathrm{d}y \\
&= \iint_{\mathbb{T}^d\times\mathbb{T}^d} e^{-im\cdot x}e^{-in\cdot y}\sum_{k\in 2\pi\mathbb{Z}^d}\widehat{w}(k)e^{ik\cdot(x-y)}\mathrm{d}x\mathrm{d}y \\
&= \sum_{k\in 2\pi\mathbb{Z}^d}\widehat{w}(k)\iint_{\mathbb{T}^d\times\mathbb{T}^d} e^{i(k-m)\cdot x}e^{i(n+k)\cdot y}\mathrm{d}x\mathrm{d}y \\
&= \sum_{k\in 2\pi\mathbb{Z}^d}\widehat{w}(k)\delta_{m=k}\delta_{n=-k} \\
&= \delta_{m=-n}\widehat{w}(n).
\end{aligned}$$

Thus Bogoliubov theory suggests that

$$H_N \approx \frac{N}{2}\widehat{w}(0) + \mathbb{H}_{\rm Bog}$$

where

$$\begin{aligned}\mathbb{H}_{\rm Bog} &= \sum_{0\neq p\in 2\pi\mathbb{Z}^d}\Big[\Big(|p|^2+\widehat{w}(p)\Big)a_p^*a_p + \frac{1}{2}\widehat{w}(p)(a_p^*a_{-p}^* + a_pa_{-p})\Big]\\ &= \frac{1}{2}\sum_{0\neq p\in 2\pi\mathbb{Z}^d}\Big[\Big(|p|^2+\widehat{w}(p)\Big)(a_p^*a_p + a_{-p}^*a_{-p}) + \widehat{w}(p)(a_p^*a_{-p}^* + a_pa_p\Big)\Big]\end{aligned}$$

As realized in Bogoliubov's 1947 paper, for any momentum $0\neq p\in 2\pi\mathbb{Z}^d$, we can "diagonalize" the summand by **completing the square**.

Exercise. *Prove that for any given parameters $A_p > B_p \geq 0$, we have*

$$A_p\Big(a_p^*a_p + a_{-p}a_{-p}\Big) + B_p(a_p^*a_{-p}^* + a_pa_{-p}) = \sqrt{A_p^2-B_p^2} - A_p + \sqrt{A_p^2-B_p^2}\,(b_p^*b_p + b_{-p}^*b_{-p})$$

where

$$b_p = a_p\sqrt{\nu_p^2+1} + a_{-p}^*\nu_p, \quad \nu_p = \sqrt{\frac{1}{2}\Big(\frac{A_p}{\sqrt{A_p^2-B_p^2}} - 1\Big)}.$$

Moreover, prove that $[b_p, b_q] = 0$ and $[b_p, b_q^*] = \delta_{p=q}$ for every $p, q\in 2\pi\mathbb{Z}^d$.

In particular, applying the above exercise with $A_p = |p|^2 + \widehat{w}(p)$ and $B_p = \widehat{w}(p)$ we obtain

$$\begin{aligned}\mathbb{H}_{\rm Bog} &= \frac{1}{2}\sum_{0\neq p\in 2\pi\mathbb{Z}^d}\Big[\Big(|p|^2+\widehat{w}(p)\Big)(a_p^*a_p + a_{-p}^*a_{-p}) + \widehat{w}(p)(a_p^*a_{-p}^* + a_pa_p\Big)\Big]\\ &= e_{\rm Bog} + \sum_{0\neq p\in 2\pi\mathbb{Z}^d} e_p b_p^* b_p\end{aligned}$$

with

$$e_{\rm Bog} = \frac{1}{2}\sum_{0\neq p\in 2\pi\mathbb{Z}^d}(\sqrt{A_p^2-B_p^2} - A_p) = \frac{1}{2}\sum_{0\neq p\in 2\pi\mathbb{Z}^d}\Big(\sqrt{|p|^4+2|p|^2\widehat{w}(p)} - |p|^2 - \widehat{w}(p)\Big)$$

and

$$e_p = \sqrt{|p|^4+2|p|^2\widehat{w}(p)}, \quad b_p = a_p\sqrt{\nu_p^2+1} + a_p^*\nu_p, \quad \nu_p = \sqrt{\frac{1}{2}\Big(\frac{|p|^2+\widehat{w}(p)}{\sqrt{|p|^4+2|p|^2\widehat{w}(p)}} - 1\Big)}.$$

In summary, for the homogeneous gas, Bogoliubov's approximation reads

$$H_N \approx \frac{N}{2}\widehat{w}(0) + e_{\rm Bog} + \sum_{0\neq p\in 2\pi\mathbb{Z}^d} e_p b_p^* b_p.$$

Note that $b_p^{\#}$'s form **new creation/annihilation operators** as they satisfy the CCR

$$[b_p, b_q] = 0, \quad [b_p^*, b_q^*] = 0, \quad [b_p, b_q^*] = \delta_{p=q}, \quad \forall p, q \in 2\pi\mathbb{Z}^d.$$

So we can treat $\sum_{0\neq p\in 2\pi\mathbb{Z}^d} e_p b_p^* b_p$ as the second quantization of a one-body operators. More precisely, we can show that there exists a unitary operator $\mathbb{U}$ (the **Bogoliubov transformation**) on the bosonic Fock space such that

$$\mathbb{U}^* a_p \mathbb{U} = b_p = a_p\sqrt{1+\nu_p^2} + a_{-p}^*\nu_p, \quad \forall 0 \neq p \in 2\pi\mathbb{Z}^d.$$

Consequently,

$$\sum_{0\neq p\in 2\pi\mathbb{Z}^d} e_p b_p^* b_p = \mathbb{U}^*\Big(\sum_{0\neq p\in 2\pi\mathbb{Z}^d} e_p a_p^* a_p\Big)\mathbb{U} = \mathbb{U}^* {\rm d}\Gamma\Big(\sum_{0\neq p\in 2\pi\mathbb{Z}^d} e_p |u_p\rangle\langle u_p|\Big)\mathbb{U}.$$

whose eigenvalues are

$$\sum_{0\neq p\in 2\pi\mathbb{Z}^d} e_p n_p, \quad n_p = 0, 1, 2, ...$$

Thus the low lying eigenvalues of H_N are of the forms

$$\frac{N}{2}\widehat{w}(0) + e_{\rm Bog} + \sum_{0\neq p\in 2\pi\mathbb{Z}^d} e_p n_p, \quad n_p = 0, 1, 2, ...$$

This calculation goes back to Bogoliubov's 1947 paper. However, this formula of the excitation spectrum was only proved rigorously in 2010 by Seiringer (CMP 2011).

In the homogeneous gas, the **diagonalization of the quadratic Hamiltonian** $\mathbb{H}_{\rm Bog}$ can be done explicitly in the level of 2×2 matrices. In order to deal with inhomogeneous trapped cases, it is important to understand **Bogoliubov transformations** in a more abstract level. This will be done in the next section.

6.3 Bogoliubov transformation

Definition. *A* **unitary operator** $\mathbb{U}$ *on the bosonic Fock space* $\mathcal{F}(\mathscr{H})$ *is called a* **Bogoliubov transformation** *if*

- *There exist bounded linear maps* $U : \mathscr{H} \to \mathscr{H}$ *and* $V : \mathscr{H}^* \to \mathscr{H}$ *such that for all* $f \in \mathscr{H}$*:*

$$\mathbb{U}^* a^*(f)\mathbb{U} = a^*(Uf) + a(VJf), \quad \mathbb{U}^* a(f)\mathbb{U} = a(Uf) + a^*(VJf),$$
$$\mathbb{U} a^*(f)\mathbb{U}^* = a^*(U^*f) - a(J^*V^*f), \quad \mathbb{U} a(f)\mathbb{U}^* = a(U^*f) - a^*(J^*V^*f).$$

- *The states* $\mathbb{U}\Omega$, $\mathbb{U}^*\Omega$ *has finite particle number expectation*

$$\langle \mathbb{U}\Omega, \mathcal{N}\mathbb{U}\Omega\rangle < \infty, \quad \langle \mathbb{U}^*\Omega, \mathcal{N}\mathbb{U}^*\Omega\rangle < \infty.$$

Example (1 dimension): Consider the case $\dim \mathscr{H} = 1$, i.e. $\mathscr{H} = \mathrm{Span}\{f\}$, $\|f\| = 1$. Then for every $\lambda \in \mathbb{R}$ the following mapping

$$\mathbb{U}_\lambda = \exp\left[\frac{\lambda}{2}(a^*(f)^2 - a(f)^2)\right]$$

is a Bogoliubov transformation on the bosonic Fock space $\mathcal{F}(\mathscr{H})$ and

$$\mathbb{U}_\lambda^* a^*(f)\mathbb{U}_\lambda = \cosh(\lambda)a^*(f) + \sinh(\lambda)a(f),$$
$$\mathbb{U}_\lambda^* a(f)\mathbb{U}_\lambda = \cosh(\lambda)a(f) + \sinh(\lambda)a^*(f).$$

In fact, since the operator

$$B = \frac{1}{2}\Big(a^*(f)^2 - a(f)^2\Big)$$

is anti-hermitian ($B^* = -B$), the mapping

$$\mathbb{U}_\lambda = e^{\lambda B}$$

is a well-defined unitary operator. Its action on the creation and annihilation operators can be computed using the Duhamel expansion and the CCR. For example when $\lambda > 0$ using

$$e^{-\lambda B}a(f)e^{\lambda B} = a(f) + \int_0^\lambda \frac{d}{dt}\Big(e^{-tB}a(f)e^{tB}\Big)\mathrm{d}t = a(f) + \int_0^\lambda e^{-tB}[a(f), B]e^{tB}\mathrm{d}t$$

and

$$[a(f), B] = \frac{1}{2}\Big(a(f)a^*(f)^2 - a^*(f)^2 a(f)\Big)$$
$$= \frac{1}{2}\Big([a(f), a^*(f)]a^*(f) + a^*(f)[a(f), a^*(f)]\Big) = a^*(f)$$

we can write

$$e^{-\lambda B} a(f) e^{\lambda B} = a(f) + \int_0^\lambda e^{-tB} a^*(f) e^{tB} \mathrm{d}t.$$

By taking the adjoint, we also obtain

$$e^{-\lambda B} a^*(f) e^{\lambda B} = a^*(f) + \int_0^\lambda e^{-tB} a(f) e^{tB} \mathrm{d}t.$$

Using repeatedly these equalities, we have the series expansion

$$\begin{aligned}
&e^{-\lambda B} a(f) e^{\lambda B} = a(f) + \int_0^\lambda e^{-tB} a^*(f) e^{tB} \mathrm{d}t \\
&= a(f) + \int_0^\lambda a^*(f)\mathrm{d}t + \int_0^\lambda \int_0^{\lambda_1} e^{-tB} a(f) e^{tB} \mathrm{d}t\mathrm{d}\lambda_1 \\
&= a(f) + \int_0^\lambda a^*(f)\mathrm{d}t + \int_0^\lambda \int_0^{\lambda_1} a(f)\mathrm{d}t\mathrm{d}\lambda_1 + \int_0^\lambda \int_0^{\lambda_1} \int_0^{\lambda_2} e^{-tB} a^*(f) e^{tB} \mathrm{d}t\mathrm{d}\lambda_2\mathrm{d}\lambda_1 \\
&= a(f) + \int_0^\lambda a^*(f)\mathrm{d}t + \int_0^\lambda \int_0^{\lambda_1} a(f)\mathrm{d}t\mathrm{d}\lambda_1 + \int_0^\lambda \int_0^{\lambda_1} \int_0^{\lambda_2} a^*(f)\mathrm{d}t\mathrm{d}\lambda_2\mathrm{d}\lambda_1 \\
&\quad + \int_0^\lambda \int_0^{\lambda_1} \int_0^{\lambda_2} \int_0^{\lambda_3} e^{-tB} a(f) e^{tB} \mathrm{d}t\mathrm{d}\lambda_3\mathrm{d}\lambda_2\mathrm{d}\lambda_1 = \dots \\
&= \sum_{n=0}^{M} \frac{\lambda^{2n}}{(2n)!} a(f) + \sum_{n=0}^{M} \frac{\lambda^{2n+1}}{(2n+1)!} a^*(f) + \int_0^\lambda \int_0^{\lambda_1} \dots \int_0^{\lambda_{2M+1}} e^{-tB} a(f) e^{tB} \mathrm{d}t\mathrm{d}\lambda_{2M+1} \dots \mathrm{d}\lambda_1.
\end{aligned}$$

Let us show that the series converges as $M \to \infty$. We have

Exercise. *Let $f \in \mathscr{H}$, $\|f\| = 1$. For every $\lambda \in \mathbb{R}$, define*

$$\mathbb{U}_\lambda = \exp\Big[\frac{\lambda}{2}(a^*(f)^2 - a(f)^2)\Big].$$

Prove the operator inequality on the bosonic Fock space $\mathcal{F}(\mathscr{H})$

$$\mathbb{U}_\lambda^*(a^*(f)a(f)+a(f)a^*(f))\mathbb{U}_\lambda \le e^{2|\lambda|}\Big(a^*(f)a(f)+a(f)a^*(f)\Big).$$

Hint: You can use Grönwall's argument.

Thus for any $\Psi \in Q(\mathcal{N}) = D(a(f))$ we have

$$\|e^{-tB}a(f)e^{tB}\Psi\| = \|a(f)e^{tB}\Psi\| = \langle \Psi, e^{-tB}a^*(f)a(f)e^{tB}\Psi\rangle^{1/2} \le e^{|t|}\Big(2\|a(f)\Psi\|^2+1\Big)^{1/2}$$

and hence

$$\begin{aligned}
&\left\| \int_0^\lambda \int_0^{\lambda_1} \dots \int_0^{\lambda_{2M+1}} e^{-tB}a(f)e^{tB}\mathrm{d}t\mathrm{d}\lambda_{2M+1}\dots\mathrm{d}\lambda_1\Psi \right\| \\
&\le \int_0^\lambda \int_0^{\lambda_1} \dots \int_0^{\lambda_{2M+1}} \|e^{-tB}a(f)e^{tB}\Psi\|\mathrm{d}t\mathrm{d}\lambda_{2M+1}\dots\mathrm{d}\lambda_1 \\
&\le C_\Psi \int_0^\lambda \int_0^{\lambda_1} \dots \int_0^{\lambda_{2M+1}} e^t\mathrm{d}t\mathrm{d}\lambda_{2M+1}\dots\mathrm{d}\lambda_1 \\
&\le C_\Psi e^\lambda \frac{\lambda^{2M+2}}{(2M+2)!} \to 0 \quad \text{ as } M\to\infty.
\end{aligned}$$

Thus in summary,

$$\begin{aligned}
e^{-\lambda B}a(f)e^{\lambda B} &= \sum_{n=0}^\infty \frac{\lambda^{2n}}{(2n)!}a(f) + \sum_{n=0}^\infty \frac{\lambda^{2n+1}}{(2n+1)!}a^*(f) \\
&= \frac{e^\lambda+e^{-\lambda}}{2}a(f) + \frac{e^\lambda - e^{-\lambda}}{2}a^*(f) \\
&= \cosh(\lambda)a(f) + \sinh(\lambda)a^*(f).
\end{aligned}$$

Thus

$$\mathbb{U}_\lambda^* a(f)\mathbb{U}_\lambda = \cosh(\lambda)a(f)+\sinh(\lambda)a^*(f), \quad \mathbb{U}_\lambda^* a^*(f)\mathbb{U}_\lambda = \cosh(\lambda)a^*(f)+\sinh(\lambda)a(f)$$

where the second identity follows from the first one by the adjointness. Since $\mathbb{U}_\lambda^* = \mathbb{U}_{-\lambda}$, we also have the reverse formula

$$\mathbb{U}_\lambda a(f)\mathbb{U}_\lambda^* = \cosh(\lambda)a(f)-\sinh(\lambda)a^*(f), \quad \mathbb{U}_\lambda a^*(f)\mathbb{U}_\lambda^* = \cosh(\lambda)a^*(f)-\sinh(\lambda)a(f).$$

Example (2 dimensions): The following example goes back to the original 1947 work of

Bogoliubov. Consider the case $\dim \mathscr{H} = 2$, i.e. $\mathscr{H} = \mathrm{Span}\{f_1, f_2\}$ with $\langle f_i, f_j\rangle = \delta_{i=j}$. For every $\lambda \in \mathbb{R}$ define

$$\mathbb{U}_\lambda = \exp\Big[\lambda(a_1^* a_2^* - a_1 a_2)\Big]$$

where $a_i = a(f_i)$ the annihilation operator. Then $\mathbb{U}_\lambda$ is a Bogoliubov transformation on the bosonic Fock space $\mathcal{F}(\mathscr{H})$ and

$$\mathbb{U}_\lambda^* a_1 \mathbb{U}_\lambda = \cosh(\lambda) a_1 + \sinh(\lambda) a_2^*, \mathbb{U}_\lambda^* a_2 \mathbb{U}_\lambda = \cosh(\lambda) a_2 + \sinh(\lambda) a_1^*.$$

These identities can be proved using the Duhamel expansion and the CCR as above. For example, when $\lambda > 0$ we can write

$$\begin{aligned}
U_\lambda^* a_1 U_\lambda &= a_1 + \int_0^\lambda \frac{d}{dt}\Big(U_t^* a_1 U_t\Big)\mathrm{d}t \\
&= a_1 + \int_0^\lambda U_t^*[a_1, a_1^* a_2^* - a_1 a_2] U_t \mathrm{d}t \\
&= a_1 + \int_0^\lambda U_t^* a_2^* U_t \mathrm{d}t \\
&= a_1 + \int_0^\lambda a_2^* \mathrm{d}t + \int_0^\lambda \int_0^{\lambda_1} U_t^* a_1 U_t \mathrm{d}t\mathrm{d}\lambda_1 \\
&= a_1 + \int_0^\lambda a_2^* \mathrm{d}t + \int_0^\lambda \int_0^{\lambda_1} a_1 \mathrm{d}t\mathrm{d}\lambda_1 + \int_0^\lambda \int_0^{\lambda_1} \int_0^{\lambda_2} U_t^* a_2^* U_t \mathrm{d}t\mathrm{d}\lambda_1\mathrm{d}\lambda_2 = \ldots \\
&= \sum_{n=0}^\infty \frac{\lambda^{2n}}{(2n)!} a_1 + \sum_{n=0}^\infty \frac{\lambda^{2n+1}}{(2n+1)!} a_2^* \\
&= \cosh(\lambda) a_1 + \sinh(\lambda) a_2^*.
\end{aligned}$$

Again, since $\mathbb{U}_\lambda^* = \mathbb{U}_{-\lambda}$, we have the reverse formula

$$\mathbb{U}_\lambda a_1 \mathbb{U}_\lambda^* = \cosh(\lambda) a_1 - \sinh(\lambda) a_2^*, \mathbb{U}_\lambda a_2 \mathbb{U}_\lambda^* = \cosh(\lambda) a_2 - \sinh(\lambda) a_1^*.$$

For future applications, we need to understand the Bogoliubov transformations on $\mathcal{F}(\mathscr{H})$ with higher dimensional cases, including the case $\dim \mathscr{H} = +\infty$. A fundamental question is under which conditions on the linear maps $U : \mathscr{H} \to \mathscr{H}$ and $V : \mathscr{H}^* \to \mathscr{H}$ we can find a Bogoliubov transformation $\mathbb{U}$ on $\mathcal{F}(\mathscr{H})$ implementing them.

The **necessary and sufficient conditions** on U and V for the existence of a Bogoliubov transformations are given by the following

Theorem (Existence of Bogoliubov transformations)**.** *The bounded linear maps* $U : \mathscr{H} \to \mathscr{H}$ *and* $V : \mathscr{H}^* \to \mathscr{H}$ *are implemented by a Bogoliubov transformation* $\mathbb{U}$ *on* $\mathcal{F}(\mathscr{H})$ **if and only if** *the following conditions hold:*

- **Shale condition:** $\mathrm{Tr}(VV^*) < \infty$.
- **Symplectic condition:**

$$UU^* - VV^* = 1 = U^*U - J^*V^*VJ, \quad U^*VJ - (U^*VJ)^* = 0 = VJU^* - (VJU^*)^*.$$

Remarks:

- In the following proof, we will deduce the Shale condition from the identity

$$\mathrm{Tr}(VV^*) = \langle \mathbb{U}\Omega, \mathcal{N}\mathbb{U}\Omega \rangle < \infty.$$

  In fact, even if we define Bogoliubov transformation without requiring $\langle \mathbb{U}\Omega, \mathcal{N}\mathbb{U}\Omega \rangle < \infty$, then the existence of Bogoliubov transformation always requires $\mathrm{Tr}(VV^*) < \infty$ (and hence implies $\langle \mathbb{U}\Omega, \mathcal{N}\mathbb{U}\Omega \rangle < \infty$ automatically). The proof of the latter point is more difficult (we do not need it).

- The "symplectic condition" can be written in a compact form with **symplectic block matrices** on $\mathscr{H} \oplus \mathscr{H}^*$

$$\mathcal{V}^*\mathcal{S}\mathcal{V} = \mathcal{V}\mathcal{S}\mathcal{V}^* = \mathcal{S},$$

  where

$$\mathcal{V} := \begin{pmatrix} U & V \\ JVJ & JUJ^* \end{pmatrix}, \quad \mathcal{S} := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

  In particular, $\mathcal{V}$ is invertible. The following exercise tells us that we can deduce one identity $VJU^* = (VJU^*)^*$ from the others.

Exercise. *Let* $U : \mathscr{H} \to \mathscr{H}$ *and* $V : \mathscr{H}^* \to \mathscr{H}$ *be bounded linear operators such that*

$$UU^* = 1 + VV^*, \quad U^*U = 1 + J^*V^*VJ, \quad U^*VJ = (U^*VJ)^*.$$

1. Prove that $VJU^* = (VJU^*)^*$*. Hint: This is equivalent to* $VJU^*UU^* = (VJU^*)^*UU^*$*.*

2. Prove that $\mathcal{V}\mathcal{S}\mathcal{V}^* = \mathcal{V}^*\mathcal{S}\mathcal{V} = \mathcal{S}$ *with*

$$\mathcal{V} := \begin{pmatrix} U & V \\ JVJ & JUJ^* \end{pmatrix}, \quad \mathcal{S} := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

3. Prove that if $\mathrm{Tr}(VV^*) < \infty$*, then* $\mathcal{V}^*\mathcal{V} - 1$ *and* $\mathcal{V}\mathcal{V}^* - 1$ *are Hilbert-Schmidt operators on* $\mathscr{H} \oplus \mathscr{H}^*$*.*

Proof of the theorem. We prove the necessity in Steps 1,2 and the sufficiency in Steps 3,4.

Part A: Necessity. We assume that there exists a Bogoliubov transformations $\mathbb{U}$ associated to U and V.

Step 1. We check the **Shale condition** $\mathrm{Tr}(VV^*) < \infty$. Let $\{f_n\}_{n\geq 1}$ be an orthonormal basis for $\mathscr{H}$. Then

$$\begin{aligned} \langle \mathbb{U}\Omega, \mathcal{N}\mathbb{U}\Omega\rangle &= \Big\langle \Omega, \mathbb{U}^* \sum_n a^*(f_n)a(f_n)\mathbb{U}\Omega \Big\rangle \\ &= \sum_n \Big\langle \Omega, \Big(a^*(Uf_n) + a(VJf_n)\Big)\Big(a(Uf_n) + a^*(VJf_n)\Big)\Omega \Big\rangle \\ &= \sum_n \Big\langle \Omega, a(VJf_n)a^*(VJf_n)\Omega \Big\rangle \\ &= \sum_n \Big\langle \Omega, \Big(a^*(VJf_n)a(VJf_n) + \|VJf_n\|^2\Big)\Omega \Big\rangle \\ &= \sum_n \|VJf_n\|^2 = \mathrm{Tr}(J^*V^*VJ) = \mathrm{Tr}(VV^*). \end{aligned}$$

Thus $\mathrm{Tr}(VV^*) = \langle \mathbb{U}\Omega, \mathcal{N}\mathbb{U}\Omega\rangle < \infty$.

Step 2. We check the **symplectic condition**. Let us introduce the **generalized annihilation and creation operators**

$$A(f \oplus Jg) = a(f) + a^*(g), \quad A^*(f \oplus Jg) = a^*(f) + a(g).$$

Then we can write the actions of the Bogoliubov transformation $\mathbb{U}$ in a compact form

$$\mathbb{U}^* A(F)\mathbb{U} = A(\mathcal{V}F), \quad \forall F \in \mathscr{H} \oplus \mathscr{H}^*.$$

On the other hand, the CCR can be rewritten as

$$[A(F), A^*(G)] = (F, \mathcal{S}G)_{\mathscr{H}\oplus\mathscr{H}^*}, \quad \forall F, G \in \mathscr{H} \oplus \mathscr{H}^*.$$

Therefore,

$$(F, \mathcal{S}G) = \mathbb{U}^*[A(F), A^*(G)]\mathbb{U} = [A(\mathcal{V}F), A^*(\mathcal{V}G)] = (\mathcal{V}F, \mathcal{S}\mathcal{V}G), \quad \forall F, G \in \mathscr{H} \oplus \mathscr{H}^*$$

which implies that

$$\mathcal{S} = \mathcal{V}^*\mathcal{S}\mathcal{V}.$$

By expanding

$$\begin{aligned}
\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} &= \begin{pmatrix} U^* & J^*V^*J^* \\ V^* & JU^*J^* \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} U & V \\ JVJ & JUJ^* \end{pmatrix} \\
&= \begin{pmatrix} U^* & J^*V^*J^* \\ V^* & JU^*J^* \end{pmatrix} \begin{pmatrix} U & V \\ -JVJ & -JUJ^* \end{pmatrix} \\
&= \begin{pmatrix} U^*U - J^*V^*VJ & U^*V - J^*V^*UJ^* \\ (U^*V - J^*V^*UJ^*)^* & V^*V - JU^*UJ^* \end{pmatrix}
\end{aligned}$$

we see that $\mathcal{V}^*\mathcal{S}\mathcal{V} = \mathcal{S}$ is equivalent to

$$U^*U = 1 + J^*V^*VJ, \quad U^*VJ = (U^*VJ)^*.$$

Similarly, using

$$\mathbb{U}A(F)\mathbb{U}^* = A(\mathcal{S}\mathcal{V}^*\mathcal{S}F), \quad \forall F \in \mathscr{H} \oplus \mathscr{H}^*$$

we find that $\mathcal{V}\mathcal{S}\mathcal{V}^* = \mathcal{S}$ which is equivalent to

$$UU^* = 1 + VV^*, \quad VJU^* = (VJU^*)^*.$$

Part B: Sufficiency. Now we assume that U and V satisfy the Shale condition $\mathrm{Tr}(VV^*) < \infty$ and the symplectic condition

$$U^*U = 1 + J^*V^*VJ, \quad UU^* = 1 + VV^*, \quad U^*VJ = (U^*VJ)^*.$$

We prove that there exists a Bogoliubov transformations $\mathbb{U}$ associated to U and V.

Step 3. We prove that there exist orthonormal bases $\{u_i\}_{i\geq 1}$ and $\{f_i\}_{i\geq 1}$ for $\mathscr{H}$ such that

$$Uu_i = \cosh(\lambda_i)f_i, \quad VJu_i = \sinh(\lambda_i)f_i, \quad \lambda_i \geq 0, \quad \forall i = 1, 2, ...$$

From the symplectic condition we know that the anti-linear operator $K = U^*VJ$ is Hermitian, i.e. $K = K^*$, and it commutes with U^*U:

$$\begin{aligned} U^*UK &= U^*UU^*VJ = U^*(1+VV^*)VJ = U^*VJ + U^*VV^*VJ \\ &= U^*VJ(1+J^*V^*VJ) = KU^*U. \end{aligned}$$

Since $U^*U - 1 = J^*V^*VJ$ is trace class (thanks to the Shale condition), U^*U has an orthonormal basis of eigenvectors. Moreover, since K commutes with U^*U, it leaves invariant eigenspaces of U^*U. Since $K = K^*$ (anti-linear Hermitian) and $K^*K = J^*V^*UU^*VJ$ is linear trace class, we can diagonalize further K on each eigenspace of U^*U (see an exercise below).

Exercise. *Let K be a bounded* **anti-linear** *map on a Hilbert-space $\mathscr{H}$. Assume that $K = K^*$, namely*

$$\langle Ku, v\rangle = \overline{\langle u, Kv\rangle} = \langle Kv, u\rangle, \quad \forall u, v \in \mathscr{H}.$$

Moreover, assume that the operator K^2 has an orthonormal eigenbasis. Prove that K has an orthonormal eigenbasis with non-negative eigenvalues.
Hint: You can write $K^2 - \lambda^2 = (K-\lambda)(K+\lambda)$.

Thus in summary, we can find an orthonormal basis $\{u_i\}_{i\ge1}$ for $\mathscr{H}$ of joint eigenvectors of U^*U and K, namely

$$U^*Uu_i = \mu_i^2 u_i, \quad Ku_i = \xi_i u_i, \quad \forall i \ge 1.$$

Here $\mu_i \ge 1$ because $U^*U \ge 1$ and $\lambda_i \ge 0$. Define $\{f_i\}$ by

$$Uu_i = \mu_i f_i, \quad \forall i \ge 1.$$

Then we have

$$\langle f_i, f_j\rangle = \mu_i^{-1}\mu_j^{-1}\langle Uu_i, Uu_j\rangle = \mu_i^{-1}\mu_j^{-1}\langle u_i, U^*Uu_j\rangle = \delta_{ij}.$$

Thus $\{f_i\}$ is an orthonormal family for $\mathscr{H}$. Moreover, if $\varphi \perp f_i$ for all i, then

$$0 = \langle \varphi, Uu_i\rangle = \langle U^*\varphi, u_i\rangle, \quad \forall i \ge 1$$

which implies that $U^*\varphi = 0$, and hence $\varphi = 0$ since $UU^* = 1 + VV^* \ge 1$ has trivial kernel. Thus $\{f_i\}$ is an orthonormal basis for $\mathscr{H}$.

On the other hand, since u_i is also eigenfunction of $K = U^*VJ$, we have

$$\langle f_j, VJu_i\rangle = \mu_j^{-1}\langle Uu_j, VJu_i\rangle = \mu_j^{-1}\langle u_j, U^*VJu_i\rangle = \mu_j^{-1}\xi_i\delta_{i=j}, \quad \forall i,j.$$

Since $\{f_i\}$ is an orthonormal basis for $\mathscr{H}$, we can use Parseval's identity

$$VJu_i = \sum_j \langle f_j, VJu_i\rangle f_j = \sum_j \mu_j^{-1}\xi_i\delta_{i=j}f_j = \nu_i f_i, \quad \nu_i := \mu_i^{-1}\xi_i \geq 0.$$

Thus we have found orthonormal bases $\{u_i\}_{i\geq 1}$ and $\{f_i\}_{i\geq 1}$ for $\mathscr{H}$ such that

$$Uu_i = \mu_i f_i, \quad VJu_i = \nu_i f_i \quad \forall i = 1,2,...$$

with $\mu_i \geq 1$ and $\nu_i \geq 0$. Moreover, $\mu_i = \sqrt{1+\nu_i^2}$ because

$$\mu_i^2 - \nu_i^2 = \|Uu_i\|^2 - \|VJu_i\|^2 = \langle u_i, (U^*U - J^*V^*VJ)u_i\rangle = \langle u_i, u_i\rangle = 1.$$

Since $\mu_i^2 - \nu_i^2 = 1$, we can write $\mu_i = \cosh(\lambda_i)$ and $\nu_i = \sinh(\lambda_i)$ for some $\lambda_i \geq 0$.

Step 4. Now we want to construct a unitary operator $\mathbb{U}$ on $\mathcal{F}(\mathscr{H})$ such that

$$\mathbb{U}^* a(u_i)\mathbb{U} = a(Uu_i) + a^*(VJu_i) = \cosh(\lambda_i)a(f_i) + \sinh(\lambda_i)a^*(f_i), \quad \forall i \geq 1.$$

This looks quite similar to the one-dimensional case that we discussed before, except that in the left side we have $a(u_i)$ instead of $a(f_i)$. More precisely, from the previous discussion on the one-dimensional case, we know that there exists a unitary operator $\widetilde{\mathbb{U}}$ on $\mathcal{F}(\mathscr{H})$ such that

$$\widetilde{\mathbb{U}}^* a(f_i)\widetilde{\mathbb{U}} = \cosh(\lambda_i)a(f_i) + \sinh(\lambda_i)a^*(f_i), \quad \forall i \geq 1.$$

In fact, $\widetilde{\mathbb{U}}$ is given by the explicit formula

$$\widetilde{\mathbb{U}} = \prod_{i\geq 1} \exp\Big(\frac{\lambda_i}{2}(a^*(f_i)^2 - a(f_i)^2)\Big) = \exp\Big(\sum_{i\geq 1}\frac{\lambda_i}{2}(a^*(f_i)^2 - a(f_i)^2)\Big).$$

Here in spite of the infinite product, or the infinite sum, the unitary operator $\widetilde{\mathbb{U}}$ is well-defined. To be precise, the condition $\mathrm{Tr}(VV^*) < \infty$ is equivalent to $\sum_{i\geq 1}\sinh(\lambda_i)^2 < \infty$, which is also equivalent to $\sum_{i\ge 1}\lambda_i^2<\infty$ (**why?**). Consequently, if we define

$$B=\sum_{i\ge 1}\frac{\lambda_i}{2}(a^*(f_i)^2-a(f_i)^2)$$

then by the Cauchy-Schwarz inequality we have the operator bound

$$\pm\mathbf{i}B\le\frac{1}{2}\sum_{i\ge 1}(a^*(f_i)a(f_i)+\lambda_i^2 a(f_i)a^*(f_i))\le\Big(1+\sum_{i\ge 1}\lambda_i^2\Big)(\mathcal{N}+1),\quad \mathbf{i}^2=-1.$$

This ensures that B is well-defined on $D(\mathcal{N})$ (a dense subset of $\mathcal{F}(\mathscr{H})$) and it is anti-hermitian ($B^*=-B$). Thus $\widetilde{\mathbb{U}}=e^B$ is a unitary operator on $\mathcal{F}(\mathscr{H})$.

Then we can choose the desired transformation $\mathbb{U}$ as

$$\mathbb{U}=\mathbb{Y}\widetilde{\mathbb{U}}$$

where $\mathbb{Y}$ is the unitary transformation on $\mathcal{F}(\mathscr{H})$ such that

$$\mathbb{Y}^*a(u_i)\mathbb{Y}=a(f_i).$$

The latter unitary operator $\mathbb{Y}$ simply corresponds to changing from the orthonormal basis

$$(n_1!n_2!...)^{-1/2}(a^*(u_1))^{n_1}(a^*(u_2))^{n_2}...\Omega,\quad n_i=0,1,2,...$$

to the orthonormal basis

$$(n_1!n_2!...)^{-1/2}(a^*(f_1))^{n_1}(a^*(f_2))^{n_2}...\Omega,\quad n_i=0,1,2,...$$

Thus we conclude that

$$\begin{aligned}\mathbb{U}^*a(u_i)\mathbb{U}&=\widetilde{\mathbb{U}}^*\mathbb{Y}^*a(u_i)\mathbb{Y}\widetilde{\mathbb{U}}=\widetilde{\mathbb{U}}^*a(f_i)\widetilde{\mathbb{U}}\\&=\cosh(\lambda_i)a(f_i)+\sinh(\lambda_i)a^*(f_i)=a(Uu_i)+a^*(VJu_i),\quad \forall i\ge 1.\end{aligned}$$

By the linearity, we obtain

$$\mathbb{U}^*a(u)\mathbb{U}=a(Uu)+a^*(VJu),\quad \forall u\in\mathscr{H}.$$

The inverse of $\mathbb{U}$ is also easy to compute. Using the property of the inverse of $\widetilde{\mathbb{U}}$ (see the one-dimensional case) and the definition of $\mathbb{Y}$, we find that

$$\begin{aligned}\mathbb{U}a(f_i)\mathbb{U}^* &= \mathbb{Y}\widetilde{\mathbb{U}}a(f_i)\widetilde{\mathbb{U}}^*\mathbb{Y}^* = \mathbb{Y}\Big(\cosh(\lambda_i)a(f_i) - \sinh(\lambda_i)\Big)\mathbb{Y}^* \\ &= \cosh(\lambda_i)a(u_i) - \sinh(\lambda_i)a^*(u_i).\end{aligned}$$

From the choice of orthonormal bases $\{u_i\}$ and $\{f_i\}$, we also find that

$$\begin{aligned}U^*f_i &= \frac{U^*Uu_i}{\|Uu_i\|} = \|Uu_i\|u_i = \cosh(\lambda_i)u_i, \\ J^*V^*f_i &= \frac{J^*V^*Uu_i}{\|Uu_i\|} = \frac{Ku_i}{\|Uu_i\|} = \sinh(\lambda_i)u_i.\end{aligned}$$

Thus

$$\mathbb{U}a(f_i)\mathbb{U}^* = \cosh(\lambda_i)a(u_i) - \sinh(\lambda_i)a^*(u_i) = a(U^*f_i) - a^*(J^*V^*f_i), \quad \forall i \geq 1$$

and hence by the linearity

$$\mathbb{U}a(f)\mathbb{U}^* = a(U^*f) - a^*(J^*V^*f), \quad \forall f \in \mathscr{H}.$$

Finally, it is easy to see that

$$\langle \mathbb{U}\Omega, \mathcal{N}\mathbb{U}\Omega\rangle = \mathrm{Tr}(VV^*) < \infty$$

and a similar bound holds for $\mathbb{U}^*\Omega$. This completes the proof of the existence of the Bogoliubov transformation. *q.e.d.*

Let us end this section by a general remark on the one-to-one correspondence between linear maps (U, V) and the set of Bogolliubov transformations (two unitary operators $\mathbb{U}$ and $z\mathbb{U}$ with $z \in \mathbb{C}$, $|z| = 1$, are considered the same).

Definition. *For a given Hilbert space $\mathscr{H}$, consider the subset of bounded linear operators on $\mathscr{H} \oplus \mathscr{H}^*$*

$$\mathscr{G} := \left\{ \mathcal{V} = \begin{pmatrix} U & V \\ JVJ & JUJ^* \end{pmatrix}, \quad \mathcal{V}^*\mathcal{S}\mathcal{V} = \mathcal{V}\mathcal{S}\mathcal{V}^* = \mathcal{S} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \mathrm{Tr}(VV^*) < \infty \right\}.$$

Remark: Equivalently

$$\mathscr{G} = \{\mathcal{V} \,|\, \mathcal{J}\mathcal{V}\mathcal{J} = \mathcal{V}, \quad \mathcal{V}^*\mathcal{S}\mathcal{V} = \mathcal{V}\mathcal{S}\mathcal{V}^* = \mathcal{S}, \quad \mathcal{V}^*\mathcal{V} - 1 \text{ is Hilbert-Schmidt}\}$$

where

$$\mathcal{J} = \begin{pmatrix} 0 & J^* \\ J & 0 \end{pmatrix}.$$

Note that $\mathcal{J}$ is a anti-linear map on $\mathscr{H} \oplus \mathscr{H}^*$ and

$$\mathcal{J} = \mathcal{J}^* = \mathcal{J}^{-1}, \quad \mathcal{J}(\mathscr{H} \oplus 0) = 0 \oplus \mathscr{H}^*.$$

Exercise. *Prove that $\mathcal{G}$ is a subgroup of the group of isomorphisms on $\mathscr{H} \oplus \mathscr{H}^*$, namely*

- *If $\mathcal{V}_1, \mathcal{V}_2 \in \mathscr{G}$, then $\mathcal{V}_1\mathcal{V}_2 \in \mathscr{G}$;*
- *If $\mathcal{V} \in \mathscr{G}$, then $\mathcal{V}^{-1} \in \mathscr{G}$.*

Exercise. *Let $\mathbb{U}_{\mathcal{V}}$ be the Bogoliubov transformation associated to $\mathcal{V} \in \mathscr{G}$.*
1. Prove that

$$\mathbb{U}_{\mathcal{V}_1}\mathbb{U}_{\mathcal{V}_2} = \mathbb{U}_{\mathcal{V}_1\mathcal{V}_2}.$$

In particular, $\mathbb{U}_{\mathcal{V}}^{-1} = \mathbb{U}_{\mathcal{V}^{-1}} = \mathbb{U}_{\mathcal{S}\mathcal{V}^*\mathcal{S}}$.
2. Prove that the set of Bogoliubov transformations is a subgroup of the group of unitary operators on $\mathcal{F}(\mathscr{H})$.

If $\mathbb{U}$ is a Bogoliubov transformation, then $\mathbb{U}^*\Omega$ can be interpreted as the **new vacuum** because it is annihilated by the **new annihilation operators**:

$$(\mathbb{U}^* a(f) \mathbb{U}) \mathbb{U}^*\Omega = \mathbb{U}^* a(f)\Omega = 0, \quad \forall f \in \mathscr{H}.$$

The explicit form of $\Omega_{\text{Bog}} = \mathbb{U}^*\Omega$ is given as follows.

Exercise. *Let $\{f_i\}$ be an orthonormal basis for $\mathscr{H}$. Let $\lambda_i \in \mathbb{R}$ such that $\sum_{i\geq 1} \lambda_i^2 < \infty$.*

Consider the state

$$\Omega_{\rm Bog} := \prod_{i\geq 1}(1-\tanh(\lambda_i)^2)^{1/4}\exp\Big(-\frac{\tanh(\lambda_i)}{2}a^*(f_i)^2\Big)\Omega.$$

Prove that $\Omega_{\rm Bog}$ *is a normalized vector in the bosonic Fock space* $\mathcal{F}(\mathscr{H})$ *and*

$$(\cosh(\lambda_i)a(f_i)+\sinh(\lambda_i)a^*(f_i))\Omega_{\rm Bog}=0, \quad \forall i\geq 1.$$

6.4 Diagonalization of block operators

Now we discuss the diagonalization of block-operators on $\mathscr{H}\oplus\mathscr{H}^*$ by symplectic operators in

$$\mathscr{G} := \left\{ \mathcal{V} = \begin{pmatrix} U & V \\ JVJ & JUJ^* \end{pmatrix}, \quad \mathcal{V}^*\mathcal{S}\mathcal{V} = \mathcal{V}\mathcal{S}\mathcal{V}^* = \mathcal{S} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \mathrm{Tr}(VV^*)<\infty \right\}.$$

The main result of this section is

Theorem (Diagonalization of bosonic block operators)**.** *Let* $h:\mathscr{H}\to\mathscr{H}$ *and* $k:\mathscr{H}^*\to\mathscr{H}$ *be linear operators satisfying*

- $h=h^*$ *(h can be unbounded);*
- $k^*=JkJ$ *and* $\mathrm{Tr}(kk^*)<\infty$*;*
- *There exists a constant* $\varepsilon_0>0$ *such that*

$$\mathcal{A} = \begin{pmatrix} h & k \\ k^* & JhJ^* \end{pmatrix} \geq \varepsilon_0 > 0 \quad \text{on } \mathscr{H}\oplus\mathscr{H}^*.$$

Then we can find an operator $\mathcal{V}\in\mathscr{G}$ *and a self-adjoint operator* $\xi>0$ *on* $\mathscr{H}$ *such that*

$$\mathcal{V}^*\mathcal{A}\mathcal{V} = \begin{pmatrix} \xi & 0 \\ 0 & J\xi J^* \end{pmatrix}.$$

If $\dim\mathscr{H}<\infty$, the result goes back to Williamson's Theorem (1936). The important case of 2×2 real matrices was solved explicitly in Bogoliubov's 1947 paper. This 2×2 case can be generalized easily to:

Example (Commutative case). Let h and k be multiplication operators on $\mathscr{H} = L^2(\Omega,\mathbb{C})$, for some measure space Ω. Then J is simply complex conjugation and we can identify $\mathscr{H}^* = \mathscr{H}$ for simplicity. Assume that $h>0$, but k is not necessarily real-valued. Then

$$\mathcal{A} := \begin{pmatrix} h & k \\ k & h \end{pmatrix} > 0 \quad \text{on } \mathscr{H}\oplus\mathscr{H}^*.$$

if and only if $-1 < G < 1$ with $G := |k|h^{-1}$. In this case, if we choose

$$\mathcal{V} := \sqrt{\frac{1}{2} + \frac{1}{2\sqrt{1-G^2}}} \begin{pmatrix} 1 & \frac{-G}{1+\sqrt{1-G^2}} \\ \frac{-G}{1+\sqrt{1-G^2}} & 1 \end{pmatrix}$$

then

$$\mathcal{V}^*\mathcal{A}\mathcal{V} = \begin{pmatrix} \xi & 0 \\ 0 & \xi \end{pmatrix} \quad \text{with} \quad \xi := h\sqrt{1-G^2} = \sqrt{h^2-k^2} > 0.$$

If $\mathcal{A} \ge \varepsilon_0 > 0$, then $h \ge \varepsilon_0 > 0$. Combining with $\mathrm{Tr}(kk^*) < \infty$ we obtain $\mathrm{Tr}(GG^*) < \infty$, which is equivalent to Shale's condition for $\mathcal{V}$.

Remark: As proved by N-Napiórkowski-Solovej (JFA 2016), the above theorem still holds true if we replace the gap condition $\mathcal{A} \ge \varepsilon_0 > 0$ and the Hilbert-Schmidt condition $\mathrm{Tr}(kk^*)$ by the weaker/optimal conditions:

$$\mathcal{A} > 0, \quad \mathrm{Tr}(h^{-1}kk^*h^{-1}) < \infty.$$

We will follow the proof of this paper.

Our starting point is a "fermionic analogue" of the above theorem.

Lemma (Diagonalization of fermionic block operators)**.** *Let $\mathcal{B}$ be a self-adjoint operator on $\mathscr{H}\oplus\mathscr{H}^*$ such that* $\mathrm{Ker}(\mathcal{B}) = \{0\}$ *and*

$$\mathcal{J}\mathcal{B}\mathcal{J} = -\mathcal{B}, \quad \mathcal{J} = \begin{pmatrix} 0 & J^* \\ J & 0 \end{pmatrix}.$$

Then there exists a unitary operator $\mathcal{U}$ on $\mathscr{H}\oplus\mathscr{H}^*$ such that $\mathcal{J}\mathcal{U}\mathcal{J} = \mathcal{U}$ and a self-adjoint operator $\xi > 0$ on $\mathscr{H}$ such that

$$\mathcal{U}^*\mathcal{B}\mathcal{U} = \begin{pmatrix} \xi & 0 \\ 0 & -J\xi J^* \end{pmatrix}$$

Remark:

- Note that $\mathcal{J}$ is a anti-linear map on $\mathscr{H} \oplus \mathscr{H}^*$ and

$$\mathcal{J} = \mathcal{J}^* = \mathcal{J}^{-1}, \quad \mathcal{J}(\mathscr{H} \oplus 0) = 0 \oplus \mathscr{H}^*.$$

- Any linear operator on $\mathscr{H} \oplus \mathscr{H}^*$ of the block form

$$\mathcal{A} = \begin{pmatrix} h & k \\ k^* & JhJ^* \end{pmatrix}, \quad k^* = JkJ, \quad h = h^*$$

  commutes with $\mathcal{J}$, namely $\mathcal{J}\mathcal{A}\mathcal{J} = \mathcal{A}$. This corresponds to **bosonic block operators**. On the other hand, in the above lemma we require that $\mathcal{B}$ anti-commutes with $\mathcal{J}$, namely $\mathcal{J}\mathcal{B}\mathcal{J} = -\mathcal{B}$, and this corresponds to **fermionic block operators**. The difference is that bosonic block operators are diagonalized by **symplectic operators**, while fermionic block operators can be diagonalized by **unitary operators** which is easier to deal with.

- The result in the above lemma also holds if $\dim \operatorname{Ker}(\mathcal{B})$ is either even or infinite (and we only know $\xi \geq 0$), but we will not need this extension.

Proof of the lemma. Since $\mathcal{B}$ is self-adjoint $\operatorname{Ker}(\mathcal{B}) = \{0\}$, by the Spectral Theorem we can decompose

$$\mathscr{H} \oplus \mathscr{H}^* = P_+ \oplus P_-$$

where

$$P_+ := \mathbb{1}(\mathcal{B} > 0)(\mathscr{H} \oplus \mathscr{H}^*), \quad P_- := \mathbb{1}(\mathcal{B} < 0)(\mathscr{H} \oplus \mathscr{H}^*).$$

The condition $\mathcal{J}\mathcal{B}\mathcal{J} = -\mathcal{B}$ implies that $P_- = \mathcal{J}P_+$. Thus we have

$$P_+ \oplus \mathcal{J}P_+ = \mathscr{H} \oplus \mathscr{H}^* = (\mathscr{H} \oplus 0) \oplus \mathcal{J}(\mathscr{H} \oplus 0).$$

The latter equality in particular implies that $\mathscr{H} \oplus 0$ and P_+ have the same dimension (finite or $+\infty$). Therefore, there exists a unitary operator $W : \mathscr{H} \oplus 0 \to P_+$. Then $\mathcal{J}W\mathcal{J} : \mathcal{J}(\mathscr{H} \oplus 0) \to \mathcal{J}P_+$ is also a unitary operator. Consequently,

$$\mathcal{U} := W \oplus \mathcal{J}W\mathcal{J}$$

is a unitary on $\mathscr{H} \oplus \mathscr{H}^*$. It is also clear from the definition of $\mathcal{U}$ that $\mathcal{J}\mathcal{U}\mathcal{J} = \mathcal{U}$.

It remains to show that $\mathcal{U}^*\mathcal{B}\mathcal{U}$ is block-diagonal. Note that for every $f \in \mathscr{H}$, we have $W(f \oplus 0) \in P_+$, and hence $\mathcal{B}W(f \oplus 0) \in P_+$, and then $W^*\mathcal{B}W(f \oplus 0) \in \mathscr{H} \oplus 0$. Thus we can define a linear operator $\xi : \mathscr{H} \to \mathscr{H}$ by

$$(\xi f) \oplus 0 := W^*\mathcal{B}W(f \oplus 0), \quad \forall f \in \mathscr{H}.$$

Note that $\xi > 0$ because

$$\langle f, \xi f \rangle = \langle f \oplus 0, (\xi f) \oplus 0 \rangle = \langle W(f \oplus 0), \mathcal{B}W(f \oplus 0) \rangle > 0 \tag{6.4.1}$$

for all $0 \neq f \in \mathscr{H}$. The last inequality follows from the facts that $W(f \oplus 0) \in P_+$ and that the restriction of $\mathcal{B}$ on P_+ is strictly positive.

We will now show that

$$\mathcal{U}^*\mathcal{B}\mathcal{U} = \begin{pmatrix} \xi & 0 \\ 0 & -J\xi J^* \end{pmatrix}$$

which is equivalent to

$$\begin{aligned} \mathcal{U}^*\mathcal{B}\mathcal{U}(f \oplus 0) &= (\xi f) \oplus 0, \\ \mathcal{U}^*\mathcal{B}\mathcal{U}(0 \oplus Jf) &= 0 \oplus (-J\xi f), \quad \forall f \in \mathscr{H}. \end{aligned}$$

Indeed, using $\mathcal{U}(f \oplus 0) = W(f \oplus 0) \in P_+$, we have $\mathcal{B}\mathcal{U}(f \oplus 0) = \mathcal{B}W(f \oplus 0) \in P_+$, and hence

$$\mathcal{U}^*\mathcal{B}\mathcal{U}(f \oplus 0) = W^*\mathcal{B}W(f \oplus 0) = (\xi f) \oplus 0.$$

Similarly, using $\mathcal{U}(0 \oplus Jf) = \mathcal{J}W\mathcal{J}(0 \oplus Jg) = \mathcal{J}W(f \oplus 0) \in P_-$, we have $\mathcal{B}\mathcal{U}(0 \oplus Jg) = \mathcal{B}\mathcal{J}W(f \oplus 0) \in P_- = \mathcal{J}P_+$, and hence

$$\begin{aligned} \mathcal{U}^*\mathcal{B}\mathcal{U}(0 \oplus Jf) &= (\mathcal{J}W^*\mathcal{J})\mathcal{B}\mathcal{J}W(f \oplus 0) = \mathcal{J}W^*(\mathcal{J}\mathcal{B}\mathcal{J})W(f \oplus 0) \\ &= -\mathcal{J}W^*\mathcal{B}W(f \oplus 0) = -\mathcal{J}((\xi f) \oplus 0) = -J\xi f. \end{aligned}$$

Here we have used $\mathcal{J}\mathcal{B}\mathcal{J} = -\mathcal{B}$. This completes the proof of the lemma. *q.e.d.*

Proof of the theorem. Since $\mathcal{A} > 0$ is self-adjoint, we can define $\mathcal{A}^{1/2} > 0$. Let us consider

$$\mathcal{B} := \mathcal{A}^{1/2}\mathcal{S}\mathcal{A}^{1/2}.$$

It is clear that $\mathcal{B}$ is self-adjoint and $\mathrm{Ker}(\mathcal{B}) = \{0\}$ because $\mathrm{Ker}(\mathcal{S}) = \mathrm{Ker}(\mathcal{A}) = \{0\}$. Moreover, $\mathcal{J}\mathcal{B}\mathcal{J} = -\mathcal{B}$ because $\mathcal{J}\mathcal{A}\mathcal{J} = \mathcal{A}$ and $\mathcal{J}\mathcal{S}\mathcal{J} = -\mathcal{S}$. By applying the result for "fermionic operators", we can find a unitary operator $\mathcal{U}$ on $\mathscr{H} \oplus \mathscr{H}^*$ such that $\mathcal{J}\mathcal{U}\mathcal{J} = \mathcal{U}$ and a self-adjoint operator $\xi > 0$ on $\mathscr{H}$ such that

$$\mathcal{U}^*\mathcal{B}\mathcal{U} = \begin{pmatrix} \xi & 0 \\ 0 & -J\xi J^* \end{pmatrix} =: D$$

Now we define

$$\mathcal{V} := \mathcal{A}^{-1/2}|\mathcal{B}|^{1/2}\mathcal{U}.$$

This choice diagonalizes $\mathcal{A}$ because

$$\mathcal{V}^*\mathcal{A}\mathcal{V} = (\mathcal{U}^*|\mathcal{B}|^{1/2}\mathcal{A}^{-1/2})\mathcal{A}(\mathcal{A}^{-1/2}|\mathcal{B}|^{1/2}\mathcal{U}) = \mathcal{U}^*|\mathcal{B}|\mathcal{U} = |\mathcal{U}^*\mathcal{B}\mathcal{U}| = |D| = \begin{pmatrix} \xi & 0 \\ 0 & J\xi J^* \end{pmatrix}.$$

Boundedness of $\mathcal{V}$. Since

$$\mathcal{A} = \begin{pmatrix} h & k \\ k^* & JhJ^* \end{pmatrix} \geq \varepsilon_0 > 0$$

and

$$\mathcal{A} - \mathcal{S}\mathcal{A}\mathcal{S} = \begin{pmatrix} h & k \\ k^* & JhJ^* \end{pmatrix} - \begin{pmatrix} h & -k \\ -k^* & JhJ^* \end{pmatrix} = 2\begin{pmatrix} 0 & k \\ k^* & 0 \end{pmatrix}$$

is bounded (because k is bounded), there exists $\delta > 0$ such that

$$\delta\mathcal{A} \leq \mathcal{S}\mathcal{A}\mathcal{S} \leq \delta^{-1}\mathcal{A}.$$

Therefore,

$$\delta\mathcal{A}^2 \leq \mathcal{B}^2 = \mathcal{A}^{1/2}\mathcal{S}\mathcal{A}\mathcal{S}\mathcal{A}^{1/2} \leq \delta^{-1}\mathcal{A}^2,$$

and hence

$$\delta^{1/2}\mathcal{A} \leq |\mathcal{B}| \leq \delta^{-1/2}\mathcal{A}.$$

In the last inequality, we have used that **the square root is operator monotone** (namely if $X \geq Y \geq 0$, then $X^{1/2} \geq Y^{1/2}$). This follows from the representation

$$X^{1/2} = \frac{2}{\pi}\int_0^\infty \frac{X}{t^2 + X}\mathrm{d}t$$

(this formula holds for real numbers $X \geq 0$, and hence it holds for self-adjoint operators $X \geq 0$ by the functional calculus) and the fact that $X \mapsto X/(X+t^2)$ is operator monotone.

Exercise. *Let X, Y be two self-adjoint operators on a Hilbert space. Prove that if $X \geq Y > 0$, then $X^{-1} \leq Y^{-1}$.*
Hint: You can use the fact that $Z^*Z \leq 1$ implies $ZZ^* \leq 1$.

Exercise. *Prove that for any power $s \in (0,1)$, the function $0 \leq t \mapsto t^s$ is operator monotone, namely if X, Y are two self-adjoint operators on a Hilbert space and $X \geq Y \geq 0$, then $X^s \geq Y^s$.*

Thus we have proved that $|\mathcal{B}| \leq \delta^{-1/2}\mathcal{A}$, which is equivalent to $(\mathcal{A}^{-1/2}|B|^{1/2})(\mathcal{A}^{-1/2}|B|^{1/2})^* = \mathcal{A}^{-1/2}|B|\mathcal{A}^{-1/2} \leq \delta^{-1/2}$. Consequently, $\mathcal{A}^{-1/2}|\mathcal{B}|^{1/2}$ is well defined on $D(|\mathcal{B}|^{1/2})$ and can be extended to be a bounded operator on $\mathscr{H} \oplus \mathscr{H}^*$. Thus $\mathcal{V} = \mathcal{A}^{-1/2}|\mathcal{B}|^{1/2}\mathcal{U}$ is well-defined as a bounded operator on $\mathscr{H} \oplus \mathscr{H}^*$.

Symplectic condition of $\mathcal{V}$. Indeed, because $\mathcal{J}$ commutes with $\mathcal{A}$, $|\mathcal{B}|$ and $\mathcal{U}$, it also commutes with $\mathcal{V}$. Thus $\mathcal{V}$ has the form

$$\mathcal{V} = \begin{pmatrix} U & V \\ JVJ & JUJ^* \end{pmatrix}.$$

Moreover, using

$$\mathcal{B} = \mathcal{A}^{1/2}\mathcal{S}\mathcal{A}^{1/2} \quad \text{and} \quad \mathcal{U}^*\mathcal{B}\mathcal{U} = \begin{pmatrix} \xi & 0 \\ 0 & -J\xi J^* \end{pmatrix} = D$$

we find that

$$\begin{aligned}
\mathcal{V}^*\mathcal{S}\mathcal{V} &= (\mathcal{U}^*|\mathcal{B}|^{1/2}\mathcal{A}^{-1/2})\mathcal{S}(\mathcal{A}^{-1/2}|\mathcal{B}|^{1/2}\mathcal{U}) \\
&= \mathcal{U}^*|\mathcal{B}|^{1/2}(\mathcal{A}^{-1/2}\mathcal{S}\mathcal{A}^{-1/2})|\mathcal{B}|^{1/2}\mathcal{U} \\
&= \mathcal{U}^*|\mathcal{B}|^{1/2}(\mathcal{B}^{-1})|\mathcal{B}|^{1/2}\mathcal{U} \\
&= |\mathcal{U}^*\mathcal{B}\mathcal{U}|^{1/2}(\mathcal{U}^*\mathcal{B}\mathcal{U})^{-1}|\mathcal{U}^*\mathcal{B}\mathcal{U}|^{1/2} = |D|^{1/2}D^{-1}|D|^{1/2} \\
&= \begin{pmatrix} \xi^{1/2} & 0 \\ 0 & J\xi^{1/2}J^* \end{pmatrix}\begin{pmatrix} \xi^{-1} & 0 \\ 0 & -J\xi^{-1}J^* \end{pmatrix}\begin{pmatrix} \xi^{1/2} & 0 \\ 0 & J\xi^{1/2}J^* \end{pmatrix}
\end{aligned}$$

$$= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \mathcal{S}$$

and

$$\begin{aligned}
\mathcal{V}\mathcal{S}\mathcal{V}^* &= (\mathcal{A}^{-1/2}|\mathcal{B}|^{1/2}\mathcal{U})\mathcal{S}(\mathcal{U}^*|\mathcal{B}|^{1/2}\mathcal{A}^{1/2}) \\
&= \mathcal{A}^{-1/2}\mathcal{U}|\mathcal{U}^*\mathcal{B}\mathcal{U}|^{1/2}\mathcal{S}|\mathcal{U}^*\mathcal{B}\mathcal{U}|^{1/2}\mathcal{U}^*\mathcal{A}^{-1/2} \\
&= \mathcal{A}^{-1/2}(\mathcal{U}|D|^{1/2}\mathcal{S}|D|^{1/2}\mathcal{U}^*)\mathcal{A}^{-1/2} \\
&= \mathcal{A}^{-1/2}\mathcal{U}D\mathcal{U}^*\mathcal{A}^{-1/2} = \mathcal{A}^{-1/2}(\mathcal{U}D\mathcal{U}^*)\mathcal{A}^{-1/2} \\
&= \mathcal{A}^{-1/2}\mathcal{B}\mathcal{A}^{-1/2} = \mathcal{A}^{-1/2}(\mathcal{A}^{1/2}\mathcal{S}\mathcal{A}^{1/2})\mathcal{A}^{-1/2} = \mathcal{S}.
\end{aligned}$$

Shale condition of $\mathcal{V}$. Finally we prove the Shale condition $\mathrm{Tr}(V^*V) < \infty$, which is equivalent to

$$\begin{aligned}
\mathcal{V}\mathcal{V}^* - 1 &= (\mathcal{A}^{-1/2}|\mathcal{B}|^{1/2}\mathcal{U})(\mathcal{U}^*|\mathcal{B}|^{1/2}\mathcal{A}^{-1/2}) - 1 \\
&= \mathcal{A}^{-1/2}|\mathcal{B}|\mathcal{A}^{-1/2} - 1 = \mathcal{A}^{-1/2}(|\mathcal{B}| - \mathcal{A})\mathcal{A}^{-1/2}
\end{aligned}$$

is a Hilbert-Schmidt operator on $\mathscr{H} \oplus \mathscr{H}^*$. Using again the representation of the square root

$$X^{1/2} = \frac{2}{\pi}\int_0^\infty \frac{X}{t^2+X}\mathrm{d}t = \frac{2}{\pi}\int_0^\infty \Big(1 - \frac{t^2}{t^2+X}\Big)\mathrm{d}t \tag{6.4.2}$$

and the resolvent identity

$$\frac{1}{t^2+\mathcal{A}^2} - \frac{1}{t^2+\mathcal{B}^2} = \frac{1}{t^2+\mathcal{A}^2}(\mathcal{B}^2-\mathcal{A}^2)\frac{1}{t^2+\mathcal{B}^2}$$

we can write

$$\begin{aligned}
\mathcal{V}\mathcal{V}^* - 1 &= \mathcal{A}^{-1/2}(|\mathcal{B}| - \mathcal{A})\mathcal{A}^{-1/2} \\
&= \frac{2}{\pi}\int_0^\infty \mathcal{A}^{-1/2}\left(\frac{1}{t^2+\mathcal{A}^2} - \frac{1}{t^2+\mathcal{B}^2}\right)\mathcal{A}^{-1/2}\, t^2\mathrm{d}t \\
&= \frac{2}{\pi}\int_0^\infty \mathcal{A}^{-1/2}\frac{1}{t^2+\mathcal{A}^2}(\mathcal{B}^2-\mathcal{A}^2)\frac{1}{t^2+\mathcal{B}^2}\mathcal{A}^{-1/2}\, t^2\mathrm{d}t \\
&= \frac{2}{\pi}\int_0^\infty \mathcal{A}^{-1/2}\frac{1}{t^2+\mathcal{A}^2}(\mathcal{A}^{1/2}\mathcal{S}\mathcal{A}\mathcal{S}\mathcal{A}^{1/2}-\mathcal{A}^2)\frac{1}{t^2+\mathcal{B}^2}\mathcal{A}^{-1/2}\, t^2\mathrm{d}t
\end{aligned}$$

$$= \frac{2}{\pi}\int_0^\infty \frac{1}{t^2+\mathcal{A}^2}(\mathcal{SAS}-\mathcal{A})\mathcal{A}^{1/2}\frac{1}{t^2+\mathcal{B}^2}\mathcal{A}^{-1/2}\,t^2\mathrm{d}t.$$

Note that

$$E := \mathcal{SAS}-\mathcal{A} = -2\begin{pmatrix} 0 & k \\ k^* & 0 \end{pmatrix}$$

is a Hilbert-Schmidt operator on $\mathscr{H}\oplus\mathscr{H}^*$. Moreover, using $\mathcal{A}\geq\varepsilon_0>0$ we can bound in the operator norm

$$\Big\|\frac{1}{t^2+\mathcal{A}^2}\Big\|_{\mathrm{op}} \leq \frac{1}{t^2+\varepsilon_0^2}.$$

Combining with $\delta^{-1}\mathcal{A}^2\geq\mathcal{B}^2\geq\delta\mathcal{A}^2$ we also have

$$\begin{aligned}\Big\|\mathcal{A}^{1/2}\frac{1}{t^2+\mathcal{B}^2}\mathcal{A}^{-1/2}\Big\|_{\mathrm{op}} &= \Big\|\mathcal{A}^{1/2}|B|^{-1/2}\frac{1}{t^2+\mathcal{B}^2}|B|^{1/2}\mathcal{A}^{-1/2}\Big\|_{\mathrm{op}}\\ &\leq \|\mathcal{A}^{1/2}|\mathcal{B}|^{-1/2}\|_{\mathrm{op}}\Big\|\frac{1}{t^2+\mathcal{B}^2}\Big\|_{\mathrm{op}}\||B|^{1/2}A^{-1/2}\|_{\mathrm{op}}\\ &\leq \frac{\delta^{-1}}{t^2+\delta\varepsilon_0^2}.\end{aligned}$$

Therefore, by the triangle inequality for the Hilbert-Schmidt norm, we find that

$$\begin{aligned}\|\mathcal{V}\mathcal{V}^*-1\|_{\mathrm{HS}} &\leq \frac{2}{\pi}\int_0^\infty \Big\|\frac{1}{t^2+\mathcal{A}^2}E\mathcal{A}^{1/2}\frac{1}{t^2+\mathcal{B}^2}\mathcal{A}^{-1/2}\Big\|_{\mathrm{HS}} t^2\mathrm{d}t\\ &\leq \frac{2}{\pi}\int_0^\infty \Big\|\frac{1}{t^2+\mathcal{A}^2}\Big\|_{\mathrm{op}}\|E\|_{\mathrm{HS}}\Big\|\mathcal{A}^{1/2}\frac{1}{t^2+B^2}\mathcal{A}^{-1/2}\Big\|_{\mathrm{op}} t^2\mathrm{d}t\\ &\leq \|E\|_{\mathrm{HS}}\cdot\frac{2}{\pi}\int_0^\infty \frac{1}{t^2+\varepsilon_0^2}\cdot\frac{\delta^{-1}}{1+\delta\varepsilon_0^2}t^2\mathrm{d}t<\infty.\end{aligned}$$

This completes the proof of the theorem. *q.e.d.*

6.5 Characterization of quasi-free states

Recall from the previous chapter that a (mixed) state G on a bosonic Fock space $\mathcal{F}(\mathscr{H})$ is a **a quasi-free state** if $\mathrm{Tr}(G\mathcal{N})<\infty$ and G satisfies Wick's Theorem, namely

$$\mathrm{Tr}(a_1^{\#}...a_{2m-1}^{\#}G)=0,\quad \forall m\geq 1$$

and

$$\mathrm{Tr}(a_1^{\#}...a_{2m}^{\#}G)=\sum_{\sigma\in P_{2m}}\mathrm{Tr}(a_{\sigma(1)}^{\#}a_{\sigma(2)}^{\#}G)...\,\mathrm{Tr}(a_{\sigma(2m-1)}^{\#}a_{\sigma(2m)}^{\#}G),\quad \forall m\geq 1.$$

A simple but very useful observation is that Bogoliubov transformations leaves invariant the set of quasi-free states.

Theorem. *Let G be a (mixed) quasi-free state on a bosonic Fock space $\mathcal{F}(\mathscr{H})$. Let $\mathbb{U}$ be a Bogoliubov transformation on $\mathcal{F}(\mathscr{H})$. Then $\mathbb{U}^*G\mathbb{U}$ is a quasi-free state.*

Proof. Recall the definition of the generalized creation/annihilation operator

$$A(f \oplus Jg) = a(f) + a^*(g), \quad \forall f, g \in \mathscr{H}.$$

Then Wick's Theorem can be rewritten as

$$\mathrm{Tr}(A(F_1)...A(F_{2m-1})G) = 0,$$

and

$$\mathrm{Tr}(A(F_1)...A(F_{2m})G) = \sum_{\sigma \in P_{2m}} \mathrm{Tr}\left[A(F_{\sigma(1)})A(F_{\sigma(2)})G\right] ... \mathrm{Tr}\left[A(F_{\sigma(2m-1)})A(F_{\sigma(2m)})G\right]$$

for all $m \geq 1$, for all vectors $F_i \in \mathscr{H} \oplus \mathscr{H}^*$ (**why?**).
On the other hand, the Bogoliubov transformation $\mathbb{U}$ acts as

$$\mathbb{U}A(F)\mathbb{U}^* = A(\mathcal{V}F), \quad \forall F \in \mathscr{H} \oplus \mathscr{H}^*$$

for some bounded linear operator $\mathcal{V}$ on $\mathscr{H} \oplus \mathscr{H}^*$,

$$\mathcal{V} = \begin{pmatrix} U & V \\ JVJ & JUJ^* \end{pmatrix}, \quad \mathcal{V}^*\mathcal{S}\mathcal{V} = \mathcal{V}\mathcal{S}\mathcal{V}^* = \mathcal{S} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \mathrm{Tr}(VV^*) < \infty.$$

Since $\mathbb{U}$ is a unitary operator, we have

$$\mathrm{Tr}(A(F_1)...A(F_n)\mathbb{U}^*G\mathbb{U}) = \mathrm{Tr}(\mathbb{U}A(F_1)...A(F_n)\mathbb{U}^*G) = \mathrm{Tr}(A(\mathcal{V}F_1)...A(\mathcal{V}F_n)G)$$

for all $n \geq 1$ and for all $F_i \in \mathscr{H} \oplus \mathscr{H}^*$. Thus we see immediately that $\mathbb{U}^*G\mathbb{U}$ also satisfies Wick's theorem. Finally,

$$\mathrm{Tr}(\mathcal{N}\mathbb{U}^*G\mathbb{U}) = \mathrm{Tr}(\mathbb{U}\mathcal{N}\mathbb{U}^*G) \leq \mathrm{Tr}(C(\mathcal{N}+1)G) < \infty.$$

q.e.d.

Exercise. *Let $\mathbb{U}$ be a Bogoliubov transformation on a bosonic Fock space $\mathcal{F}(\mathscr{H})$. Prove that for every $k \in \mathbb{N}$, there exists a constant $C = C(k, \mathbb{U})$ such that we have the operator inequality on Fock space*

$$\mathbb{U}^*(\mathcal{N}+1)^k\mathbb{U} \leq C(\mathcal{N}+1)^k.$$

Next, let us consider the relation between quasi-free states and their generalized one-body density matrices. From the definition, it is obvious that any quasi-free state G is determined completely by its generalized one-body density matrix

$$\Gamma_G := \begin{pmatrix} \gamma_G & \alpha_G \\ \alpha_G^* & 1 + J\gamma_G J^* \end{pmatrix}.$$

Recall also that $\Gamma_G \geq 0$, $\alpha_G^* = J\alpha_G J$ and $\operatorname{Tr}\gamma_G < \infty$.

Now we are able to prove the full one-to-one correspondence between quasi-free states and its generalized one-body density matrices.

Theorem. *Consider a bounded linear operator on $\mathscr{H} \oplus \mathscr{H}^*$*

$$\Gamma := \begin{pmatrix} \gamma & \alpha \\ \alpha^* & 1 + J\gamma J^* \end{pmatrix} \geq 0$$

with $\alpha^* = J\alpha J$ and $\operatorname{Tr}\gamma < \infty$. Then there exists **a unique (mixed) quasi-free state** *G on the bosonic Fock space $\mathcal{F}(\mathscr{H})$ such that $\Gamma = \Gamma_G$, the generalized one-body density matrix of G.*

Proof. **Step 1.** We will apply the previous theorem to

$$\mathcal{A} := \Gamma + \frac{1}{2}\mathcal{S} = \begin{pmatrix} \gamma + \frac{1}{2} & \alpha \\ \alpha^* & \frac{1}{2} + J\gamma J^* \end{pmatrix}.$$

We have $\mathcal{J}\mathcal{A}\mathcal{J} = \mathcal{A}$. Moreover, recall that the condition $\Gamma \geq 0$ is equivalent to

$$\gamma \geq J^*\alpha^*(1+\gamma)^{-1}\alpha J \text{ on } \mathscr{H}$$

which in particular implies that

$$\mathrm{Tr}(\alpha\alpha^*) \le (1+\|\gamma\|_{\mathrm{op}})\,\mathrm{Tr}(\gamma) < \infty.$$

Also, $\mathcal{A} \ge 0$ since

$$\Gamma = \begin{pmatrix} \gamma & \alpha \\ \alpha^* & 1+J\gamma J^* \end{pmatrix} \ge 0, \quad \Gamma + \mathcal{S} = \begin{pmatrix} \gamma+1 & \alpha \\ \alpha^* & J\gamma J^* \end{pmatrix} = \mathcal{J}\Gamma\mathcal{J} \ge 0.$$

By a refined analysis, we can show that $\mathcal{A} \ge \varepsilon_0 > 0$.

Exercise. *Prove that there exists a constant* $\varepsilon_0 > 0$ *such that* $\mathcal{A} \ge \varepsilon_0 > 0$.
Hint: $\mathrm{Ker}(\mathcal{A}) = \mathrm{Ker}(\Gamma) \cap \mathrm{Ker}(\Gamma+\mathcal{S}) = \{0\}$ *and* $\mathcal{A} - \frac{1}{2}$ *is Hilbert-Schmidt.*

Thus we can diagonalize $\mathcal{A}$ by a block operator $\mathcal{V} \in \mathscr{G}$, namely

$$\mathcal{V}^*\mathcal{A}\mathcal{V} = \begin{pmatrix} \xi & 0 \\ 0 & J\xi J^* \end{pmatrix}$$

with a self-adjoint operator $\xi > 0$ on $\mathscr{H}$ and

$$\mathcal{V} = \begin{pmatrix} U & V \\ JVJ & JUJ^* \end{pmatrix}, \quad \mathcal{V}^*\mathcal{S}\mathcal{V} = \mathcal{V}\mathcal{S}\mathcal{V}^* = \mathcal{S}, \quad \mathrm{Tr}(VV^*) < \infty.$$

Step 2. We have

$$\mathcal{V}^*\Gamma\mathcal{V} = \mathcal{V}^*\mathcal{A}\mathcal{V} - \frac{1}{2}\mathcal{V}^*\mathcal{S}\mathcal{V} = \mathcal{V}^*\mathcal{A}\mathcal{V} - \frac{1}{2}\mathcal{S} = \begin{pmatrix} \xi' & 0 \\ 0 & 1+J\xi' J^* \end{pmatrix}$$

with $\xi' = \xi - \frac{1}{2}$. Since $\Gamma \ge 0$, we find that $\mathcal{V}^*\Gamma\mathcal{V} \ge 0$, and hence $\xi' \ge 0$.

Let us show that ξ' is trace class. In principle, we can compute ξ' directly by expanding $\mathcal{V}^*\Gamma\mathcal{V}$. However, here we represent another proof which is more useful later. We observe that

$$\begin{aligned} \Gamma\mathcal{S}(\Gamma+\mathcal{S}) &= \begin{pmatrix} \gamma & \alpha \\ \alpha^* & 1+J\gamma J^* \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1+\gamma & \alpha \\ \alpha^* & J\gamma J^* \end{pmatrix} \\ &= \begin{pmatrix} \gamma(\gamma+1) - \alpha\alpha^* & \gamma\alpha - \alpha J\gamma J^* \\ \alpha^*\gamma - J\gamma J^*\alpha^* & \alpha^*\alpha - J\gamma(\gamma+1)J^* \end{pmatrix} \end{aligned}$$

is a trace class operator on $\mathscr{H} \oplus \mathscr{H}^*$. Combining with

$$\mathcal{V}^*\Gamma\mathcal{V} = \begin{pmatrix} \xi' & 0 \\ 0 & 1 + J\xi' J^* \end{pmatrix}, \quad \mathcal{V}^*(\Gamma + \mathcal{S})\mathcal{V} = \mathcal{V}^*\Gamma\mathcal{V} + \mathcal{S} = \begin{pmatrix} 1+\xi' & 0 \\ 0 & J\xi' J^* \end{pmatrix}$$

we find that

$$\begin{aligned} \mathcal{V}^*\Gamma S(\Gamma + S)\mathcal{V} &= \mathcal{V}^*\Gamma(\mathcal{V}\mathcal{S}\mathcal{V}^*)(\Gamma + S)\mathcal{V} = (\mathcal{V}^*\Gamma\mathcal{V})\mathcal{S}(\mathcal{V}^*(\Gamma + S)\mathcal{V}) \\ &= \begin{pmatrix} \xi' & 0 \\ 0 & 1 + J\xi' J^* \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 1+\xi' & 0 \\ 0 & J\xi' J^* \end{pmatrix} \\ &= \begin{pmatrix} \xi'(1+\xi') & 0 \\ 0 & -J\xi'(1+\xi')J^* \end{pmatrix} \end{aligned}$$

is a trace class operator on $\mathscr{H} \oplus \mathscr{H}^*$. Consequently, $\xi'(1+\xi')$ is a trace class operator on $\mathscr{H}$, and hence ξ' is a trace class operator on $\mathscr{H}$.

Step 3. Let us show that there exists a (mixed) quasi-free state G' on $\mathcal{F}(\mathscr{H})$ whose generalized one-body density matrix is

$$\Gamma_{G'} = \begin{pmatrix} \xi' & 0 \\ 0 & 1 + J\xi' J^* \end{pmatrix} = \mathcal{V}^*\Gamma\mathcal{V}.$$

Simple case. Let us consider the case $\xi' > 0$ for simplicity. Then we can define

$$h := \log\left(1 + (\xi')^{-1}\right)$$

by Spectral Theorem, namely if

$$\xi' = \sum_n \lambda_n |u_n\rangle\langle u_n|, \quad \{u_n\} \text{ an orthonormal basis}, \quad \lambda_1 \geq \lambda_2 \geq ... > 0,$$

then

$$h = \sum_n \log\left(1 + \lambda_n^{-1}\right)|u_n\rangle\langle u_n|.$$

Note that

$$\operatorname{Tr} e^{-h} = \operatorname{Tr}\left[\left(1 + (\xi')^{-1}\right)^{-1}\right] = \operatorname{Tr}\left[\frac{\xi'}{1+\xi'}\right] \leq \operatorname{Tr}\xi' < \infty.$$

Thus we can simply take G' the Gaussian state

$$G' := Z_0^{-1} e^{-\mathrm{d}\Gamma(h)} = Z_0^{-1} \exp\Big[-\sum_n \log\Big(1+\lambda_n^{-1}\Big) a^*(u_n)a(u_n)\Big], \quad Z_0 = \mathrm{Tr}\, e^{-\mathrm{d}\Gamma(h)}.$$

Recall from the computation for Gaussian states, we know that $\alpha_{G'} = 0$ and

$$\gamma_{G'} = \frac{1}{e^h - 1} = \frac{1}{e^{\log(1+(\xi')^{-1})} - 1} = \frac{1}{\Big(1+(\xi')^{-1}\Big) - 1} = \xi'.$$

Thus the generalized one-body density matrix of the Gaussian state G' is exactly

$$\Gamma_{G'} = \begin{pmatrix} \xi' & 0 \\ 0 & 1 + J\xi' J^* \end{pmatrix}.$$

General case. It remains to consider the general case $\xi' \geq 0$. Again we write

$$\xi' = \sum_n \lambda_n |u_n\rangle\langle u_n|, \quad \{u_n\} \text{ an orthonormal basis}, \quad \lambda_1 \geq \lambda_2 \geq ... \geq 0.$$

For any $M \geq 2$, define

$$\xi'_M := \sum_n (\lambda_n + M^{-n}) |u_n\rangle\langle u_n|.$$

Then $\xi'_M > 0$ is a trace class operator on $\mathscr{H}$. The corresponding Gaussian state

$$\begin{aligned} G'_M &:= Z_M^{-1} \exp\Big[-\mathrm{d}\Gamma\Big(\log\big(1 + (\xi'_M)^{-1}\big)\Big)\Big] \\ &= Z_M^{-1} \exp\Big[-\sum_n \log\Big(1 + (\lambda_n + M^{-n})^{-1}\Big) a^*(u_n)a(u_n)\Big] \end{aligned}$$

has the one-body density matrix $\gamma_{G'_M} = \xi'_M$. Then we can check that

$$G' := \lim_{M\to\infty} G'_M$$

exists in trace class and it is a quasi-free state with

$$\Gamma_{G'} = \lim_{M\to\infty} \Gamma_{G'_M} = \begin{pmatrix} \xi' & 0 \\ 0 & 1 + J\xi' J^* \end{pmatrix}.$$

Exercise. *Consider the Gaussian states G'_M as above.*

1. Prove that the partition function Z_M converges to a limit $Z_0 \in (0,\infty)$ as $M \to \infty$.

2. Prove that $G'_M \to G'$ strongly in trace class.

3. Prove that G' is a quasi-free state and

$$G' = Z_0^{-1} \exp\Big[- \sum_{n\in I} \log\Big(1+\lambda_n^{-1}\Big) a^*(u_n)a(u_n)\Big]\Pi_0$$

where $I = \{n : \lambda_n > 0\}$ and Π_0 is the orthogonal projection onto $\mathrm{Ker}\Big(\sum_{n\notin I} a^*(u_n)a(u_n)\Big)$.
Hint: You can use Monotone Convergence.

Step 4. We have constructed a quasi-free state G' such that $\Gamma_{G'} = \mathcal{V}^*\Gamma\mathcal{V}$. Now we construct a quasi-free state G such that $\Gamma_G = \Gamma$.

Since $\mathcal{V} \in \mathscr{G}$, there exists a Bogoliubov transformation $\mathbb{U}$ such that

$$\mathbb{U}^* A(F)\mathbb{U} = A(\mathcal{V}F), \quad \forall F \in \mathscr{H} \oplus \mathscr{H}^*.$$

Here recall that

$$A(f \oplus Jg) = a(f) + a^*(g), \quad \forall f, g \in \mathscr{H}.$$

We choose

$$G := \mathbb{U}^* G' \mathbb{U}.$$

Since G' is a quasi-free state and Bogoliubov transformations leave invariant the set of quasi-free states, G is also a quasi-free state. It remains to show that $\Gamma_G = \Gamma$.
We have the following general fact.

Exercise. *Let G' be an arbitrary mixed state on the bosonic Fock space $\mathcal{F}(\mathscr{H})$ with $\mathrm{Tr}(\mathcal{N}G') < \infty$. Let $\mathbb{U}$ be a Bogoliubov transformation and $\mathcal{V}$ the corresponding block operator on $\mathscr{H} \oplus \mathscr{H}^*$, namely*

$$\mathbb{U}^* A(F)\mathbb{U} = A(\mathcal{V}F), \quad \forall F \in \mathscr{H} \oplus \mathscr{H}^*.$$

Prove that $\mathcal{V}^*\Gamma_G\mathcal{V} = \Gamma_{G'}$ with $G = \mathbb{U}^* G' \mathbb{U}$.
Hint: You can use $\mathrm{Tr}\Big[A^*(F_1)A(F_2)G\Big] = \langle F_2, \Gamma_G F_1\rangle, \quad \forall F_1, F_2 \in \mathscr{H} \oplus \mathscr{H}^*$.

Thus we deduce that, with $G = \mathbb{U}^* G' \mathbb{U}$

$$\mathcal{V}^* \Gamma_G \mathcal{V} = \Gamma_{G'} = \begin{pmatrix} \xi' & 0 \\ 0 & 1 + J\xi' J^* \end{pmatrix} = \mathcal{V}^* \Gamma \mathcal{V}.$$

This implies that $\Gamma_G = \Gamma$ since $\mathcal{V}$ is invertible. *q.e.d.*

Finally, we turn to

Theorem (Pure quasi-free states)**.** *Any pure state $G = |\Psi\rangle\langle\Psi|$ on the bosonic Fock space $\mathcal{F}(\mathscr{H})$ is a quasi-free state* **if and only if** *$\Psi = \mathbb{U}\Omega$ with a Bogolliubov transformation $\mathbb{U}$. Moreover, any bounded linear operator on $\mathscr{H} \oplus \mathscr{H}^*$*

$$\Gamma := \begin{pmatrix} \gamma & \alpha \\ \alpha^* & 1 + J\gamma J^* \end{pmatrix} \geq 0, \quad \alpha^* = J\alpha J, \quad \operatorname{Tr} \gamma < \infty$$

is the generalized one-body density matrix of a pure quasi-free state **if and only if**

$$\Gamma \mathcal{S} \Gamma = -\Gamma.$$

The latter condition is equivalent to $\gamma(\gamma + 1) = \alpha\alpha^*$ and $\gamma\alpha J = \alpha J \gamma$.

Proof. **Step 1.** Since $|\Omega\rangle\langle\Omega|$ is a (trivial) quasi-free state and any Bogoliubov transformation $\mathbb{U}$ leaves invariant the set of quasi-free states, we know that $|\mathbb{U}\Omega\rangle\langle\mathbb{U}\Omega|$ is also a quasi-free state (and it is a pure state).

The reverse direction is less trivial. Recall from the proof of the previous theorem, for any (mixed) quasi-free state G we can find a Bogoliubov transformation $\mathbb{U}$ such that

$$\mathbb{U}^* G \mathbb{U} = Z_0^{-1} \exp\Big[-\sum_{n \in I} \Big(1 + \lambda_n^{-1}\Big) a^*(u_n) a(u_n) \Big] \Pi_0$$

where $\{u_n\}_n$ is an orthonormal basis for $\mathscr{H}$, $I = \{n : \lambda_n > 0\}$, and Π_0 the orthogonal projection onto $\operatorname{Ker}(\sum_{n \notin I} a^*(u_n) a(u_n))$. In particular, if $G = |\Psi\rangle\langle\Psi|$ is a pure state, then $\mathbb{U}^* G \mathbb{U}$ is also a pure state. In this case

$$\mathbb{U}^* G \mathbb{U} = (\mathbb{U}^* G \mathbb{U})^2 = Z_0^{-2} \exp\Big[-\sum_{n \in I} 2\Big(1 + \lambda_n^{-1}\Big) a^*(u_n) a(u_n) \Big] \Pi_0.$$

If $I \neq \emptyset$, then clearly

$$Z_0^{-1} \exp\Big[-\sum_{n\in I}\Big(1+\lambda_n^{-1}\Big)a^*(u_n)a(u_n)\Big], \quad Z_0^{-2} \exp\Big[-\sum_{n\in I}2\Big(1+\lambda_n^{-1}\Big)a^*(u_n)a(u_n)\Big]$$

are two different Gaussian states on the sub-Fock space

$$\mathcal{F}(\mathrm{Span}(u_n : n \in I))$$

and hence we get a contradiction. Thus if $G = |\Psi\rangle\langle\Psi|$ is a pure quasi-free state, then we must have $I = \emptyset$. Thus $\mathbb{U}^* G \mathbb{U} = \Pi_0$ with Π_0 the orthogonal projection onto $\bigcap_{n\notin I} \mathrm{Ker}(a^*(u_n)a(u_n)) = \mathrm{Ker}(\mathcal{N})$, namely

$$\mathbb{U}^*|\Psi\rangle\langle\Psi| = \mathbb{U}^* G \mathbb{U} = \Pi_0 = |\Omega\rangle\langle\Omega|.$$

Equivalently,

$$|\Psi\rangle\langle\Psi| = \mathbb{U}|\Omega\rangle\langle\Omega|\mathbb{U}^* = |\mathbb{U}\Omega\rangle\langle\mathbb{U}\Omega|$$

which means that Ψ is equal to $\mathbb{U}\Omega$, up to a phase factor.

Step 2. Next, let us consider the generalized one-body density matrix. Recall from the proof of the previous theorem, any bounded linear operator on $\mathscr{H} \oplus \mathscr{H}^*$

$$\Gamma := \begin{pmatrix} \gamma & \alpha \\ \alpha^* & 1 + J\gamma J^* \end{pmatrix} \geq 0, \quad \alpha^* = J\alpha J, \quad \mathrm{Tr}\,\gamma < \infty$$

is the generalized one-body density matrix of (mixed) quasi-free state G; more precisely, there exists a Bogoliubov transformation $\mathbb{U}$ and a corresponding block operator $\mathcal{V} \in \mathscr{G}$, i.e.

$$\mathbb{U}^* A(F) \mathbb{U} = A(\mathcal{V}F), \quad \forall F \in \mathscr{H} \oplus \mathscr{H}^*,$$

such that $G = \mathbb{U}^* G' \mathbb{U}$ and

$$\Gamma_{G'} = \mathcal{V}^* \Gamma \mathcal{V} = \begin{pmatrix} \xi' & 0 \\ 0 & 1 + J\xi' J^* \end{pmatrix}$$

where $\xi' \geq 0$ is a trace class operator on $\mathscr{H}$. Recall that as we argued before, the latter formula of $\mathcal{V}^*\Gamma\mathcal{V}$ implies that

$$\mathcal{V}^*\Gamma\mathcal{S}(\Gamma + \mathcal{S})\mathcal{V} = \begin{pmatrix} \xi'(1+\xi') & 0 \\ 0 & -J\xi'(1+\xi')J^* \end{pmatrix}$$

In particular, the fact that G is a pure quasi-free state is equivalent to $G' = |\Omega\rangle\langle\Omega|$, which is equivalent to $\xi' = 0$, and also equivalent to $\Gamma\mathcal{S}(\Gamma + \mathcal{S}) = 0$, namely $\Gamma\mathcal{S}\Gamma = -\Gamma$. From the explicit computation

$$\Gamma\mathcal{S}(\Gamma+\mathcal{S}) = \begin{pmatrix} \gamma(\gamma+1) - \alpha\alpha^* & \gamma\alpha - \alpha J\gamma J^* \\ \alpha^*\gamma - J\gamma J^*\alpha^* & \alpha^*\alpha - J\gamma(\gamma+1)J^* \end{pmatrix}$$

we see that $\Gamma\mathcal{S}(\Gamma+\mathcal{S}) = 0$ means two equalities

$$\gamma(\gamma+1) = \alpha\alpha^*, \quad \gamma\alpha J = \alpha J\gamma.$$

q.e.d.

6.6 Diagonalization of quadratic Hamiltonians

Definition. *A* **quadratic Hamiltonian** *on the bosonic Fock space $\mathcal{F}(\mathscr{H})$ is a linear operator which is quadratic in terms of creation and annihilation operators*

$$\mathbb{H} = \mathrm{d}\Gamma(h) + \frac{1}{2}\sum_{m,n\geq 1}\Big(\langle u_m, kJu_n\rangle a^*(u_m)a^*(u_n) + \overline{\langle u_m, kJu_n\rangle} a(u_m)a(u_n)\Big)$$

with a self-adjoint operator $h : \mathscr{H} \to \mathscr{H}$ and a linear operator $k : \mathscr{H}^* \to \mathscr{H}$ satisfying $k^* = JkJ$. Here $\{u_n\}$ is an orthonormal basis for $\mathscr{H}$.

Theorem (Diagonalization of quadratic Hamiltonians)**.** *Let h be self-adjoint on $\mathscr{H}$, $k : \mathscr{H}^* \to \mathscr{H}$ be linear such that $k^* = JkJ$ and $\mathrm{Tr}(kk^*) < \infty$. Moreover,*

$$\mathcal{A} := \begin{pmatrix} h & k \\ k^* & JhJ^* \end{pmatrix} \geq \varepsilon_0 > 0 \quad \text{on } \mathscr{H} \oplus \mathscr{H}^*.$$

Then the followings hold true for the quadratic Hamiltonian $\mathbb{H}$ associated to h and k:

- *$\mathbb{H}$ is well-defined on the core domain*

$$\bigcup_{M\geq 0}\Big(\bigoplus_{n=0}^{M} D(h)^{\otimes_s n}\Big) \subset \mathcal{F}(\mathscr{H}).$$

Moreover, $\mathbb{H}$ is bounded from below

$$\mathbb{H} \geq -\frac{1}{2}\operatorname{Tr}(k^*h^{-1}k)$$

and can be extended to be a self-adjoint operator on $\mathcal{F}(\mathscr{H})$ by Friedrichs' method.

- *There exists a Bogoliubov transformation $\mathbb{U}$ on $\mathcal{F}(\mathscr{H})$ and a self-adjoint operator $\xi > 0$ on $\mathscr{H}$ such that*
$$\mathbb{U}^*\mathbb{H}\mathbb{U} = \mathrm{d}\Gamma(\xi) + \inf\sigma(\mathbb{H}).$$
- *The unique ground state of $\mathbb{H}$ (up to a phase factor) is the pure quasi-free state $\mathbb{U}\Omega$ and*
$$\inf\sigma(\mathbb{H}) = \operatorname{Tr}(h\gamma_{\mathbb{U}\Omega}) + \Re\operatorname{Tr}(k^*\alpha_{\mathbb{U}\Omega}).$$

Proof. **Step 1.** First we prove that the quadratic form of $\mathbb{H}$ can be represented in terms of the generalized one-body density matrices. In fact, for any "reasonable" state $\Psi \in \mathcal{F}(\mathscr{H})$ we have

$$\langle\Psi, \mathbb{H}\Psi\rangle = \operatorname{Tr}(h\gamma_\Psi) + \Re\operatorname{Tr}(k^*\alpha_\Psi).$$

Recall the definition of one-body density matrices

$$\langle g, \gamma_G f\rangle_{\mathscr{H}} = \langle\Psi, a^*(f)a(g)\Psi\rangle, \quad \langle g, \alpha_\Psi Jf\rangle = \langle\Psi, a(f)a(g)\Psi\rangle.$$

We have, at least formally,

$$\begin{aligned}
\langle\Psi, \mathrm{d}\Gamma(h)\Psi\rangle &= \sum_{m,n\geq 1}\langle u_m, hu_n\rangle\langle\Psi, a^*(u_m)a(u_n)\Psi\rangle \\
&= \sum_{m,n\geq 1}\langle u_m, hu_n\rangle\langle u_n, \gamma_\Psi u_m\rangle = \sum_{n\geq 1}\Big\langle u_n, \gamma_\Psi\sum_m\langle u_m, hu_n\rangle u_m\Big\rangle \\
&= \sum_{n\geq 1}\Big\langle u_n, \gamma_\Psi hu_n\Big\rangle = \operatorname{Tr}(\gamma_\Psi h) = \operatorname{Tr}(h\gamma_\Psi) \quad (= \operatorname{Tr}(\gamma_\Psi^{1/2}h\gamma_\Psi^{1/2}))
\end{aligned}$$

and

$$\begin{aligned}
&\Big\langle\Psi, \Big(\frac{1}{2}\sum_{m,n\geq 1}\Big(\langle u_m, kJu_n\rangle a^*(u_m)a^*(u_n) + \overline{\langle u_m, kJu_n\rangle}a(u_m)a(u_n)\Big)\Psi\Big\rangle \\
&= \Re\sum_{m,n\geq 1}\overline{\langle u_m, kJu_n\rangle}\langle\Psi, a(u_m)a(u_n)\Psi\rangle = \Re\sum_{m,n\geq 1}\overline{\langle u_m, kJu_n\rangle}\langle u_m, \alpha_\Psi Ju_n\rangle
\end{aligned}$$

$$
\begin{aligned}
&= \Re \sum_{n\geq 1} \Big\langle \sum_{m\geq 1} \langle u_m, kJu_n\rangle u_m, \alpha_\Psi J u_n \Big\rangle = \Re \sum_{n\geq 1} \Big\langle kJu_n, \alpha_\Psi J u_n \Big\rangle \\
&= \Re \sum_{n\geq 1} \Big\langle Ju_n, k^* \alpha_\Psi J u_n \Big\rangle = \mathrm{Tr}(k^* \alpha_\Psi).
\end{aligned}
$$

The above calculation can be made rigorous for example if Ψ belongs to the core domain

$$
\mathcal{Q} := \bigcup_{M\geq 0} \Big(\bigoplus_{n=0}^{M} D(h)^{\otimes_s n} \Big) \subset \mathcal{F}(\mathscr{H}).
$$

Indeed, if $\mathrm{Tr}(\mathcal{N}G) < \infty$, then $\mathrm{Tr}(\gamma_\Psi) < \infty$ and $\mathrm{Tr}(\alpha_\Psi \alpha_\Psi^*) < \infty$, and hence $\mathrm{Tr}(k^*\alpha_\Psi)$ is finite, while $\mathrm{Tr}(h\gamma_\Psi)$ is well-defined (can be $+\infty$, but always $> -\infty$).

Step 2. Now we prove that $\mathbb{H}$ is bounded from below. Recall that from $\Gamma_\Psi \geq 0$ we have

$$
\gamma_\Psi \geq \alpha_\Psi J (1+\gamma_\Psi)^{-1} J^* \alpha_\Psi^*
$$

By the same reasoning, from $\mathcal{A} \geq 0$ we find that

$$
h \geq kJh^{-1}J^*k^* = J^*k^*h^{-1}kJ.
$$

Using the cyclicity of the trace and the Cauchy-Schwarz inequality we can estimate

$$
\begin{aligned}
|\mathrm{Tr}(k^*\alpha_\Psi)| &= |\mathrm{Tr}((1+\gamma_\Psi)^{1/2} J^* k^* h^{-1/2} \cdot h^{1/2} \alpha_\Psi J (1+\gamma_\Psi)^{-1/2})| \\
&\leq \|(1+\gamma_\Psi)^{1/2} J^* k^* h^{-1/2}\|_{\mathrm{HS}} \cdot \|h^{1/2}\alpha_\Psi J(1+\gamma_\Psi)^{-1/2}\|_{\mathrm{HS}}.
\end{aligned}
$$

Since

$$
\begin{aligned}
\|(1+\gamma_\Psi)^{1/2} J^* k^* h^{-1/2}\|_{\mathrm{HS}} &= \sqrt{\mathrm{Tr}\left((1+\gamma_\Psi)^{1/2} J^* k^* h^{-1} kJ (1+\gamma_\Psi)^{1/2} \right)} \\
&= \sqrt{\mathrm{Tr}(k^* h^{-1} k) + \mathrm{Tr}\left(J^* k^* h^{-1} kJ \gamma_\Psi \right)} \leq \sqrt{\mathrm{Tr}(k^* h^{-1} k) + \mathrm{Tr}\left(h\gamma_\Psi \right)}
\end{aligned}
$$

and

$$
\|h^{1/2}\alpha_\Psi J(1+\gamma_\Psi)^{-1/2}\|_{\mathrm{HS}} = \sqrt{\mathrm{Tr}\left(h^{1/2}\alpha_\Psi J (1+\gamma_\Psi)^{-1} J^* \alpha_\Psi^* h^{1/2} \right)} \leq \sqrt{\mathrm{Tr}\left(h\gamma_\Psi \right)}
$$

we find that

$$\begin{aligned}|\operatorname{Tr}(k^*\alpha_\Psi)| &\le \sqrt{\operatorname{Tr}(h^{1/2}\gamma_\Psi h^{1/2})}\cdot\sqrt{\operatorname{Tr}(kh^{-1}k^*)+\operatorname{Tr}(h^{1/2}\gamma_\Psi h^{1/2})}\\ &\le \operatorname{Tr}(h^{1/2}\gamma_\Psi h^{1/2})+\frac{1}{2}\operatorname{Tr}(kh^{-1}k^*).\end{aligned}$$

Here in the last estimate we have used the elementary inequality

$$\sqrt{x(x+y)}=\sqrt{(x+y/2)^2-y^2/4}\le x+y/2,\quad \forall x,y\in[0,\infty).$$

Combining with Step 1, we conclude that for any $\Psi\in\mathcal{Q}$,

$$\langle\Psi,\mathbb{H}\Psi\rangle=\operatorname{Tr}(h\gamma_\Psi)+\Re\operatorname{Tr}(k^*\alpha_\Psi)\ge-\frac{1}{2}\operatorname{Tr}(kh^{-1}k^*).$$

Thus $\mathbb{H}$ is bounded from below and it can be extended to be a self-adjoint operator by Friedrichs' method. The extension, still denoted by $\mathbb{H}$, satisfies

$$\mathbb{H}\ge-\frac{1}{2}\operatorname{Tr}(kh^{-1}k^*).$$

Step 3. Finally we prove that $\mathbb{H}$ can be diagonalized by a Bogoliubov transformation.

Finite dimensional case. To make the argument transparent, let us first consider the case when $\mathscr{H}$ is finite dimensional. Using the calculation in Step 1, we can connect the quadratic Hamiltonian $\mathbb{H}$ on $\mathcal{F}(\mathscr{H})$ and the block operator $\mathcal{A}$ on $\mathscr{H}\oplus\mathscr{H}^*$ as follows:

$$\begin{aligned}\langle\Psi,\mathbb{H}\Psi\rangle=\operatorname{Tr}(h\gamma_\Psi)+\Re\operatorname{Tr}(k^*\alpha_\Psi)&=\frac{1}{2}\operatorname{Tr}\left[\begin{pmatrix}h & k\\ k^* & JhJ^*\end{pmatrix}\begin{pmatrix}\gamma_\Psi & \alpha_\Psi\\ \alpha_\Psi^* & J\gamma_\Psi J^*\end{pmatrix}\right]\\ &=\frac{1}{2}\operatorname{Tr}(\mathcal{A}\Gamma_\Psi)-\frac{1}{2}\operatorname{Tr}h.\end{aligned}$$

By the assumptions on $\mathcal{A}$, we know that there exists a block operator $\mathcal{V}\in\mathscr{G}$ which diagonalizes $\mathcal{A}$, namely

$$\mathcal{V}\mathcal{A}\mathcal{V}^*=\begin{pmatrix}\xi & 0\\ 0 & J\xi J^*\end{pmatrix}$$

for some self-adjoint operator $\xi>0$ on $\mathscr{H}$. Now let $\mathbb{U}$ be the corresponding Bogoliubov transformation, namely

$$\mathbb{U}^*A(F)\mathbb{U}=A(\mathcal{V}F),\quad \forall F\in\mathscr{H}\oplus\mathscr{H}^*.$$

Then recall from a previous exercise that

$$\Gamma_{\mathbb{U}\Psi} = \mathcal{V}^* \Gamma_\Psi \mathcal{V}.$$

Thus for any pure state $\Psi \in \mathcal{F}(\mathscr{H})$ we have

$$\begin{aligned}
\langle \Psi, \mathbb{U}^* \mathbb{H} \mathbb{U} \Psi \rangle = \langle \mathbb{U}\Psi, \mathbb{H}\mathbb{U}\Psi\rangle &= \frac{1}{2}\operatorname{Tr}(\mathcal{A}\Gamma_{\mathbb{U}\Psi}) - \frac{1}{2}\operatorname{Tr} h \\
&= \frac{1}{2}\operatorname{Tr}(\mathcal{A}\mathcal{V}^*\Gamma_\Psi\mathcal{V}) - \frac{1}{2}\operatorname{Tr} h = \frac{1}{2}\operatorname{Tr}(\mathcal{V}\mathcal{A}\mathcal{V}^*\Gamma_\Psi) - \frac{1}{2}\operatorname{Tr} h \\
&= \frac{1}{2}\operatorname{Tr}\left[\begin{pmatrix} \xi & 0 \\ 0 & J\xi J^* \end{pmatrix}\begin{pmatrix} \gamma_\Psi & \alpha_\Psi \\ \alpha_\Psi^* & 1 + J\gamma_\Psi J^* \end{pmatrix}\right] - \frac{1}{2}\operatorname{Tr} h \\
&= \operatorname{Tr}(\xi\gamma_\Psi) + \frac{1}{2}\operatorname{Tr}(\xi) - \frac{1}{2}\operatorname{Tr}(h) \\
&= \langle \Psi, \mathrm{d}\Gamma(\xi)\Psi\rangle + \frac{1}{2}\operatorname{Tr}(\xi - h).
\end{aligned}$$

This means that $\mathbb{U}$ diagonalizes $\mathbb{H}$, namely

$$\mathbb{U}^*\mathbb{H}\mathbb{U} = \mathrm{d}\Gamma(\xi) + \frac{1}{2}\operatorname{Tr}(\xi - h).$$

Note that $\mathrm{d}\Gamma(\xi) \geq 0$, with 0 is the lowest eigenvalue with Ω the unique eigenvector. Therefore, $\mathbb{H}$ has the unique ground state $\mathbb{U}\Omega$, with the ground state energy $\inf \sigma(\mathbb{H}) = \frac{1}{2}\operatorname{Tr}(\xi - h)$.

General case. The proof in the general case follows a similar strategy, except that we cannot write $\operatorname{Tr}(\xi) - \operatorname{Tr}(h)$ since ξ and h can be not trace class separately.
As in above, let $\mathcal{V} \in \mathscr{G}$ be the block operator diagonalizing $\mathcal{A}$:

$$\mathcal{V}\mathcal{A}\mathcal{V}^* = \begin{pmatrix} \xi & 0 \\ 0 & J\xi J^* \end{pmatrix}$$

for some self-adjoint operator $\xi > 0$ on $\mathscr{H}$. To proceed in the infinite dimensional case, we need

Lemma. *If $\mathcal{V} \in \mathscr{G}$ and $\mathcal{V}\mathcal{A}\mathcal{V}^*$ is block diagonal, then*

$$\mathcal{V}^*\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}\mathcal{V} = \begin{pmatrix} X & Y \\ Y^* & 1 + JXJ^* \end{pmatrix}$$

where $X \geq 0$ with $X^{1/2}hX^{1/2}$ a trace class operator on $\mathscr{H}$ and $\mathrm{Tr}(YY^*) < \infty$.

Let $\mathbb{U}$ be the corresponding Bogoliubov transformation, namely

$$\mathbb{U}^* A(F)\mathbb{U} = A(\mathcal{V}F), \quad \forall F \in \mathscr{H} \oplus \mathscr{H}.$$

Then for any state $\Psi \in \mathcal{F}(\mathscr{H})$ we can write

$$\Gamma_{\mathbb{U}\Psi} = \mathcal{V}^*\Gamma_\Psi\mathcal{V} = \mathcal{V}^* \begin{pmatrix} \gamma_\Psi & \alpha_\Psi \\ \alpha_\Psi^* & 1 + J\gamma_\Psi J^* \end{pmatrix} \mathcal{V} = \mathcal{V}^* \begin{pmatrix} \gamma_\Psi & \alpha_\Psi \\ \alpha_\Psi^* & J\gamma_\Psi J^* \end{pmatrix} \mathcal{V} + \begin{pmatrix} X & Y \\ Y^* & 1 + JXJ^* \end{pmatrix}.$$

Consequently,

$$\begin{pmatrix} \gamma_{\mathbb{U}\Psi} & \alpha_{\mathbb{U}\Psi} \\ \alpha_{\mathbb{U}\Psi}^* & J\gamma_{\mathbb{U}\Psi}J^* \end{pmatrix} = \mathcal{V}^* \begin{pmatrix} \gamma_\Psi & \alpha_\Psi^* \\ \alpha_\Psi & J\gamma_\Psi J^* \end{pmatrix} \mathcal{V} + \begin{pmatrix} X & Y \\ Y^* & JXJ^* \end{pmatrix}.$$

Therefore, combining with the computation in Step 1, we have

$$\begin{aligned}
\langle \Psi, \mathbb{U}^*\mathbb{H}\mathbb{U}\Psi\rangle = \langle \mathbb{U}\Psi, \mathbb{H}\mathbb{U}\Psi\rangle &= \mathrm{Tr}(h\gamma_{\mathbb{U}\Psi}) + \Re\,\mathrm{Tr}(k^*\alpha_{\mathbb{U}\Psi}) = \frac{1}{2}\mathrm{Tr}\left[\mathcal{A}\begin{pmatrix} \gamma_{\mathbb{U}\Psi} & \alpha_{\mathbb{U}\Psi} \\ \alpha_{\mathbb{U}\Psi}^* & J\gamma_{\mathbb{U}\Psi}J^* \end{pmatrix}\right] \\
&= \frac{1}{2}\mathrm{Tr}\left[\mathcal{A}\mathcal{V}^*\begin{pmatrix} \gamma_\Psi & \alpha_\Psi \\ \alpha_\Psi^* & J\gamma_\Psi J^* \end{pmatrix}\mathcal{V}\right] + \frac{1}{2}\mathrm{Tr}\left[\mathcal{A}\begin{pmatrix} X & Y \\ Y^* & JXJ^* \end{pmatrix}\right] \\
&= \frac{1}{2}\mathrm{Tr}\left[\begin{pmatrix} \xi & 0 \\ 0 & J\xi J^* \end{pmatrix}\begin{pmatrix} \gamma_\Psi & \alpha_\Psi \\ \alpha_\Psi^* & J\gamma_\Psi J^* \end{pmatrix}\right] + \frac{1}{2}\mathrm{Tr}\left[\begin{pmatrix} h & k \\ k^* & JhJ^* \end{pmatrix}\begin{pmatrix} X & Y \\ Y^* & JXJ^* \end{pmatrix}\right] \\
&= \mathrm{Tr}(\xi\gamma_\Psi) + \mathrm{Tr}(hX) + \Re\,\mathrm{Tr}(k^*Y) \\
&= \langle \Psi, \mathrm{d}\Gamma(\xi)\Psi\rangle + \mathrm{Tr}(hX) + \Re\,\mathrm{Tr}(k^*Y).
\end{aligned}$$

Thus

$$\mathbb{U}^*\mathbb{H}\mathbb{U} = \mathrm{d}\Gamma(\xi) + \mathrm{Tr}(hX) + \Re\,\mathrm{Tr}(k^*Y).$$

Here note that $\gamma_{\mathbb{U}\Omega} = X$ and $\alpha_{\mathbb{U}\Omega} = Y$. Thus we obtain the desired conclusion. *q.e.d.*

It remains to prove the above technical lemma.

Proof of the lemma. Let $U : \mathscr{H} \to \mathscr{H}$ and $V : \mathscr{H}^* \to \mathscr{H}$ be the block components of $\mathcal{V}$. Then we can write

$$\mathcal{V}^*\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}\mathcal{V} = \begin{pmatrix} U^* & J^*V^*J^* \\ V^* & JU^*J^* \end{pmatrix}\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} U & V \\ JVJ & JUJ^* \end{pmatrix} = \begin{pmatrix} X & Y \\ Y^* & 1 + JXJ^* \end{pmatrix}$$

where

$$X = J^*V^*VJ \geq 0, \quad Y = J^*V^*UJ^*.$$

Thanks to Shale's condition $\mathrm{Tr}(VV^*) < \infty$ we obtain immediately

$$\mathrm{Tr}(X) < \infty, \quad \mathrm{Tr}(YY^*) < \infty.$$

Now we prove that $\mathrm{Tr}(X^{1/2}hX^{1/2}) < \infty$, using the additional information that $\mathcal{V}\mathcal{A}\mathcal{V}^*$ is block diagonal. By a straightforward computation of the off-diagonal term of

$$\mathcal{V}\mathcal{A}\mathcal{V}^* = \begin{pmatrix} U & V \\ JVJ & JUJ^* \end{pmatrix} \begin{pmatrix} h & k \\ k^* & JhJ^* \end{pmatrix} \begin{pmatrix} U^* & J^*V^*J^* \\ V^* & JU^*J^* \end{pmatrix}$$

we find that

$$UhJ^*V^* + UkJU^* + Vk^*J^*V^* + VJhU^* = 0.$$

Recall from the proof of the existence of Bogoliubov transformations, we can find orthonormal bases $\{u_i\}_{i\geq 1}$, $\{f_i\}_{i\geq 1}$ for $\mathscr{H}$ and $\lambda_i \geq 0$ such that

$$U^*u_i = \cosh(\lambda_i)f_i, \quad J^*V^*u_i = \sinh(\lambda_i)f_i, \quad \forall i \geq 1.$$

(If we change $\mathcal{V} \mapsto \mathcal{V}^*$, then $(U, VJ) \mapsto (U^*, J^*V^*)$). Consequently,

$$\begin{aligned} 0 &= \langle u_i, (UhJ^*V^* + UkJU^* + Vk^*J^*V^* + VJhU^*)u_i\rangle \\ &= 2\cosh(\lambda_i)\sinh(\lambda_i)\langle f_i, hf_i\rangle + \cosh(\lambda_i)^2\langle f_i, kJf_i\rangle + \sinh(\lambda_i)^2\langle f_i, J^*k^*f_i\rangle \end{aligned}$$

and hence

$$2\cosh(\lambda_i)\sinh(\lambda_i)\langle f_i, hf_i\rangle = -(\cosh(\lambda_i)^2 + \sinh(\lambda_i)^2)\langle f_i, kJf_i\rangle, \quad \forall i \geq 1.$$

On the other hand, since $\{u_i\}$ are eigenfunctions of UU^*, $\{f_i\}$ are eigenfunctions of U^*U:

$$U^*Uf_i = \frac{U^*UU^*f_i}{\|U^*u_i\|} = \frac{U^*u_i\|U^*u_i\|^2}{\|U^*u_i\|} = f_i\|U^*u_i\|^2 = \cosh(\lambda_i)^2 f_i, \quad \forall i \geq 1.$$

Combining with $U^*U = 1 + J^*V^*VJ = 1 + X$ we find that

$$Xf_i = (\cosh(\lambda_i)^2 - 1)f_i = \sinh(\lambda_i)^2 f_i, \quad \forall i \geq 1.$$

Consequently, from the above computations and the Cauchy-Schwarz inequality we have

$$\begin{aligned}
\operatorname{Tr}(X^{1/2}hX^{1/2}) &= \sum_{i\geq 1}\langle f_i, X^{1/2}hX^{1/2}f_i\rangle = \sum_{i\geq 1}\sinh(\lambda_i)^2\langle f_i, hf_i\rangle \\
&= -\sum_{i\geq 1}\frac{\sinh(\lambda_i)}{2\cosh(\lambda_i)}(\cosh(\lambda_i)^2+\sinh(\lambda_i)^2)\langle f_i, kJf_i\rangle \\
&\leq \Big[\sum_{i\geq 1}\Big(\frac{\sinh(\lambda_i)}{2\cosh(\lambda_i)}(\cosh(\lambda_i)^2+\sinh(\lambda_i)^2)\Big)^2\Big]^{1/2}\Big[\sum_{i\geq 1}|\langle f_i, kJf_i\rangle|^2\Big]^{1/2} \\
&\leq \Big[\sum_{i\geq 1}\sinh(\lambda_i)^2\sup_j(1+2\sinh(\lambda_j)^2)^2\Big]^{1/2}\Big[\sum_{i\geq 1}\|kJf_i\|^2\Big]^{1/2} \\
&\leq \Big[\operatorname{Tr}(VV^*)(1+2\operatorname{Tr}(VV^*))^2\Big]^{1/2}\Big[\operatorname{Tr}(kk^*)\Big]^{1/2} < \infty.
\end{aligned}$$

Thus $X^{1/2}hX^{1/2}$ is trace class. This completes the proof of the lemma. *q.e.d.*

Chapter 7

Validity of Bogoliubov approximation

In this chapter we will rigorously justify Bogoliubov's approximation for weakly interacting Bose gases. We focus on the **mean-field regime** where the system contains N identical bosons in $\mathbb{R}^d$, described by the Hamilttonian

$$H_N = \sum_{i=1}^{N}(-\Delta_{x_i} + V(x_i)) + \frac{1}{N-1}\sum_{1\le i<j\le N} w(x_i - x_j)$$

acting on $L^2(\mathbb{R}^d)^{\otimes_s N}$. Let us think of the simple situation with

- **Trapping potential:** $V \in L^\infty_{\rm loc}(\mathbb{R}^d,\mathbb{R})$, $\lim_{|x|\to\infty} V(x) = +\infty$;
- **Positive-type bounded interaction:** $0 \le \widehat{w} \in L^1(\mathbb{R}^d)$.

(More general conditions will be discussed later.) Then we know that there exists a unique Hartree minimizer $u_0 \ge 0$ and there is the complete Bose-Einstein condensation, namely

- **The ground state energy** of H_N is given by the Hartree energy to the leading order

  $$E_N = Ne_{\rm H} + \mathcal{O}(1)$$

  where

  $$e_{\rm H} := \inf_{\|u\|_{L^2(\mathbb{R}^d)}=1}\Big(\int |\nabla u(x)|^2 {\rm d}x + \int V(x)|u(x)|^2{\rm d}x + \frac{1}{2}\iint |u(x)|^2|u(y)|^2 w(x-y){\rm d}x{\rm d}y\Big).$$

- **The approximate ground states** $\langle \Psi_N, H_N \Psi_N \le Ne_{\rm H} + \mathcal{O}(1)$ safisfies

  $$\langle u_0, \gamma^{(1)}_{\Psi_N} u_0\rangle = N + \mathcal{O}(1).$$

In this chapter, we will prove that

$$E_N = Ne_{\rm H} + e_{\rm Bog} + o(1)$$

where $e_{\rm Bog}$ is the ground state energy of a **quadratic Hamiltonian** $\mathbb{H}_{\rm Bog}$ on Fock space which is predicted by Bogoliubov's approximation. More generally, we will show that the n-th eigenvalue of H_N is

$$\mu_n(H_N) = Ne_{\rm H} + \mu_n(\mathbb{H}_{\rm Bog}) + o(1), \quad \forall n = 1, 2, ...$$

We also obtain the convergence of the eigenstates for H_N in terms of the Hartree minimizer u_0 (the condensate) and the eigenstates of $\mathbb{H}_{\rm Bog}$ (excited particles).

These results were first proved by Seiringer (2010) for the homogeneous gas and by Grech-Seiringer (2013) for trapped gases (the setting we consider here). We will follow the approach by Lewin-N-Serfaty-Solovej (CPAM 2015), with some simplifications.

7.1 Bogoliubov Hamiltonian

Bogoliubov's theory suggests that the excited particles (particles outside of the condensation) are described by the **quadratic Hamiltonian**

$$\mathbb{H}_{\rm Bog} = \sum_{m,n\ge 1} \langle u_m, (h+K)u_n\rangle a_m^* a_n + \frac{1}{2}\sum_{m,n\ge 1}\Big(\langle u_m, KJu_n\rangle a_m^* a_n^* + h.c.\Big)$$

where

- $\{u_n\}_{n=0}^\infty$ is an orthonormal basis for $\mathscr{H} = L^2(\mathbb{R}^d)$; given $u_0 \ge 0$ we can take all u_n's of real-valued functions;
- h is the mean-field operator associated to the Hartree equation

  $$h = -\Delta + V + |u_0|^2 * w - \mu, \quad hu_0 = 0;$$

  Recall that $h \ge 0$ and u_0 is the unique ground state for h on $\mathscr{H}$. Moreover, the condition $V(x) \to +\infty$ as $|x| \to \infty$ ensures that h has compact resolvent. In particular, we have the **spectral gap**

  $$h \ge \varepsilon_0 > 0 \quad \text{ on } \mathscr{H}_+ := \{u_0\}^\perp.$$

- $K : \mathscr{H} \to \mathscr{H}$ is a linear operator with kernel

$$K(x,y) = u_0(x)u_0(y)w(x-y).$$

  The condition $\widehat{w} \geq 0$ implies that K is a positive operator on $\mathscr{H}$ (**why**?).

Note that we will think of $\mathbb{H}_{\rm Bog}$ as an operator on the **excited Fock space**

$$\mathcal{F}(\mathscr{H}_+) = \mathbb{C} \oplus \mathscr{H}_+ \oplus \mathscr{H}_+^{\otimes_s 2} \oplus ..., \quad \mathscr{H}_+ = \{u_0\}^\perp = Q\mathscr{H}, \quad Q = 1 - |u_0\rangle\langle u_0|.$$

Theorem. *The Bogoliubov Hamiltonian $\mathbb{H}_{\rm Bog}$ on the excited Fock space $\mathcal{F}(\mathscr{H}_+)$ is a self-adjoint operator with the same quadratic form domain of $\mathrm{d}\Gamma(h)_{|\mathcal{F}(\mathscr{H}_+)}$. Moreover,*

- *There exist a Bogoliubov transformation $\mathbb{U}$ on $\mathcal{F}(\mathscr{H}_+)$ and a self-adjoint operator $\xi > 0$ on $\mathscr{H}_+$ with compact resolvent such that*

$$\mathbb{U}^* \mathbb{H}_{\rm Bog} \mathbb{U} = \mathrm{d}\Gamma(\xi) + e_{\rm Bog}.$$

- *The ground state energy is finite*

$$e_{\rm Bog} := \inf \sigma(\mathbb{H}_{\rm Bog}) \in (-\infty, 0].$$

  Moreover, $\mathbb{H}_{\rm Bog}$ has a unique ground state $\mathbb{U}\Omega$ (up to a complex phase). This ground state is a pure quasi-free state on $\mathcal{F}(\mathscr{H}_+)$.

- *$\mathbb{H}_{\rm Bog}$ has compact resolvent and its spectrum is*

$$\sigma(\mathbb{H}_{\rm Bog}) = \Big\{ e_{\rm Bog} + \sum_{i=1}^\infty n_i e_i \,|\, e_i \in \sigma(\xi), n_i = 0,1,2,... \Big\}.$$

Remark: The ground state energy $e_{\rm Bog}$ is always negative (< 0) except the non-interacting case ($w = 0$).

Proof. First, let us rewrite the Bogoliubov Hamiltonian in a form compatible to the previous chapter. It is convenient to restrict the relevant operators h, K to the subspace $\mathscr{H}_+$. Since $hu_0 = 0$, h leaves invariant $\mathscr{H}_+$ and we will still denote by h the restriction to $\mathscr{H}_+$. Recall that

$$\inf \sigma(h_{|\mathscr{H}_+}) > 0,$$

Moreover, using $Q = 1 - |u_0\rangle\langle u_0|$ we define $K_1 : \mathscr{H}_+ \to \mathscr{H}_+$ and $K_2 : \mathscr{H}_+^* \to \mathscr{H}_+$ by

$$K_1 := QKQ, \quad K_2 = QKJQJ^*.$$

$$\mathbb{H}_{\rm Bog} = \sum_{m,n\ge 1} \langle u_m, (h+K_1)u_n\rangle a_m^* a_n + \frac{1}{2}\sum_{m,n\ge 1}\Big(\langle u_m, K_2 J u_n\rangle a_m^* a_n^* + h.c.\Big)$$

Then $K_1^* = K_1$, $K_2^* = JK_2J^*$ and both K_1, K_2 are Hilbert-Schmidt operators. Using the positivity of $\widehat{w}$, we can deduce that $K_1 \ge 0$, and hence $h + K_1 > 0$. Moreover, we have the positivity of the block operator on $\mathscr{H}_+ \oplus \mathscr{H}_+^*$.

Exercise. *Prove the operator inequality on* $\mathscr{H}_+ \oplus \mathscr{H}_+^*$

$$\mathcal{A} := \begin{pmatrix} h+K_1 & K_2 \\ K_2^* & J(h+K_1)J^* \end{pmatrix} \ge \inf \sigma(h) > 0.$$

Thus by the results in the previous chapter, we can find a block operator $\mathcal{V} \in \mathscr{G}$ and a self-adjoint operator ξ on $\mathscr{H}_+$ such that

$$\mathcal{V}\mathcal{A}\mathcal{V}^* = \begin{pmatrix} \xi & 0 \\ 0 & J\xi J^* \end{pmatrix}.$$

Moreover, the corresponding Bogoliubov transformation $\mathbb{U}$ diagonalizes $\mathbb{H}_{\rm Bog}$ on $\mathcal{F}(\mathscr{H}_+)$:

$$\mathbb{U}^* \mathbb{H} \mathbb{U} = {\rm d}\Gamma(\xi) + e_{\rm Bog}.$$

In particular, $\mathbb{H}_{\rm Bog}$ can be defined as a self-adjoint operator on $\mathcal{F}(\mathscr{H}_+)$ and it is bounded from below:

$$e_{\rm Bog} = \inf \sigma(\mathbb{H}_{\rm Bog}) \ge -\frac{1}{2}{\rm Tr}_{\mathscr{H}_+}(K_2^*(h+K_1)^{-1}K_2) > -\infty.$$

Since h has compact resolvent, ξ also has compact resolvent. So it has eigenvalues $0 < e_1 \le e_2 \le ...$ and $\lim_{n\to\infty} e_n = +\infty$. The spectrum of $\mathbb{H}_{\rm Bog}$ is

$$\sigma(\mathbb{H}_{\rm Bog}) = e_{\rm Bog} + \sigma({\rm d}\Gamma(\xi)) = \Big\{ e_{\rm Bog} + \sum_i n_i e_i \,|\, n_i = 0,1,2,... \Big\}.$$

q.e.d.

7.2 Unitary implementing c-number substitution

Heuristically, the Bogoliubov approximation can be interpreted as

$$H_N - Ne_{\mathrm{H}} \approx \mathbb{H}_{\mathrm{Bog}}.$$

However, this formulation is a bit formal since the operators $H_N - E_N$ and $\mathbb{H}_{\mathrm{Bog}}$ live in different Hilbert space. This incompatibility comes from the c-number substitution which replace a_0, a_0^* (which does not preserve the particle number) by $\sqrt{N_0}$ (which preserves the particle number).

To resolve this problem, we an operator U_N from the N-body Hilbert space $\mathscr{H}^{\otimes_s N}$ to the **excited Fock space** $\mathcal{F}(\mathscr{H}_+)$. We start with a useful observation

$$\mathcal{F}(\mathscr{H}) = \mathcal{F}(P\mathscr{H} \oplus Q\mathscr{H}) \cong \mathcal{F}(P\mathscr{H}) \otimes \mathcal{F}(Q\mathscr{H}).$$

with $P = |u_0\rangle\langle u_0|$, $Q = 1 - P$. Consequently, for any wave function $\Psi \in \mathscr{H}^{\otimes_s N}$, we can write uniquely as

$$\Psi := \varphi_0 \, u_0^{\otimes N} + u_0^{\otimes(N-1)} \otimes_s \varphi_1 + u_0^{\otimes(N-2)} \otimes_s \varphi_2 + \cdots + \varphi_N$$

where $\varphi_k \in \mathscr{H}_+^{\otimes_s^k}$. To be precise, we have

Definition. *Let u_0 be a normalized vector in a Hilbert space $\mathscr{H}$. Let $\mathscr{H}_+ = \{u_0\}^\perp \subset \mathscr{H}$ and $a_0 = a(u_0)$. We define the operator $U_N = U_N(u_0)$,*

$$U_N : \mathscr{H}^{\otimes_s N} \to \mathcal{F}^{\leq N}(\mathscr{H}_+) = \mathbb{C} \oplus \mathscr{H}_+ \oplus \mathscr{H}_+^{\otimes_s 2} \oplus \cdots \oplus \mathscr{H}_+^{\otimes_s N}$$

by

$$U_N \Psi = \bigoplus_{j=0}^{N} Q^{\otimes j} \Big(\frac{a_0^{N-j}}{\sqrt{(N-j)!}} \Psi \Big).$$

Theorem. *The operator* $U_N : \mathscr{H}^{\otimes_s N} \to \mathcal{F}^{\leq N}(\mathscr{H}_+)$ *is a* **unitary operator** *with*

$$U_N^* : \mathcal{F}^{\leq N}(\mathscr{H}_+) \to \mathscr{H}^{\otimes_s N}, \quad U_N^*\Big(\bigoplus_{j=0}^{N} \varphi_j\Big) = \sum_{j=0}^{N} \frac{(a_0^*)^{N-j}}{\sqrt{(N-j)!}} \varphi_j$$

Moreover, we have the operator identities on $\mathcal{F}^{\leq N}(\mathscr{H}_+)$ *for all* $m, n \neq 0$

$$U_N a_0^* a_0 U_N^* = N - \mathcal{N}_+, \quad U_N a_m^* a_n U_N^* = a_m^* a_n,$$
$$U_N a_0^* a_n U_N^* = \sqrt{N - \mathcal{N}_+}\, a_n, \quad U_N a_n^* a_0 U_N^* = a_n^* \sqrt{N - \mathcal{N}_+}$$

where $a_n = a(u_n)$ *and* $u_m, u_n \in \mathscr{H}_+$ *when* $m, n \neq 0$.

Remarks:

- The number operator $\mathcal{N}_+$ on $\mathcal{F}(\mathscr{H}_+) = \mathcal{F}(Q\mathscr{H}_+)$ is equal to $\mathcal{N}_{|\mathcal{F}(\mathscr{H}_+)}$, the restriction of the number operator $\mathcal{N} = \mathrm{d}\Gamma(1)$ on $\mathcal{F}(\mathscr{H})$ to the subspace $\mathcal{F}(\mathscr{H}_+) \subset \mathcal{F}(\mathscr{H})$. We have the operator identities on $\mathcal{F}(\mathscr{H})$:

$$\mathcal{N}_+ = \mathrm{d}\Gamma(Q) = \mathcal{N} - a^*(u_0) a(u_0).$$

For any wave function $\Psi_N \in \mathscr{H}^{\otimes_s N}$, we have

$$\langle u_0, \gamma^{(1)}_{\Psi_N} u_0 \rangle = \langle \Psi_N, a^*(u_0) a(u_0) \Psi_N \rangle = N - \langle \Psi_N, \mathcal{N}_+ \Psi_N \rangle.$$

Therefore, the Bose-Einstein condensation $\langle u_0, \gamma^{(1)}_{\Psi_N} u_0 \rangle = N + o(N)$ is equivalent to

$$\langle \Psi_N, \mathcal{N}_+ \Psi_N \rangle \ll N.$$

- Roughly speaking, the transformation $U_N(\cdot)U_N^*$ **replaces** $a(u_0), a^*(u_0)$ **by** $\sqrt{N - \mathcal{N}_+}$. Thanks to the Bose-Einstein condensation, we can think of the operator $\sqrt{N - \mathcal{N}_+}$ as the scalar number $\sqrt{N}$. Thus the unitary operator U_N provides a rigorous way to formulate the **c-number substitution** in Bogoliubov's argument.

- Recall that the Weyl operator

$$W := W(\sqrt{N} u_0) = \exp\Big(\sqrt{N}(a_0^* - a_0)\Big)$$

satisfies

$$W^* a_0 W = a_0 + \sqrt{N}, \quad W^* a_0^* W = a_0^* + \sqrt{N}, \quad W^* a_n W = a_n, \quad n \neq 0.$$

Thus U_N looks similar to the Weyl operator. However, while the Weyl operator is defined on the full Fock space $\mathcal{F}(\mathscr{H})$, the operator U_N is more appropriate to work on the N-particle space $\mathscr{H}^{\otimes_s N}$. Unlike the Weyl operator, we can only write $U_N a^*(f) a(g) U_N^*$ but it suffices for applications ($U_N a(f) U_N^*$ makes no sense).

- By definition $U_N^* : \mathcal{F}^{\leq N}(\mathscr{H}_+) \to \mathscr{H}^{\otimes_s N}$. However, we can extend U_N^* to the full excited Fock space $\mathcal{F}^{\leq N}(\mathscr{H}_+)$ by setting 0 outside $\mathcal{F}^{\leq N}(\mathscr{H}_+)$. This extension makes U_N a **partial isometry** from $\mathscr{H}^{\otimes_s N}$ to $\mathcal{F}^{\leq N}(\mathscr{H}_+)$.

Proof of the theorem. **Part I.** We will prove that

$$U_N^* : \mathcal{F}^{\leq N}(\mathscr{H}_+) \to \mathscr{H}^{\otimes_s N}, \quad U_N^* \Big(\bigoplus_{j=0}^{N} \varphi_j \Big) = \sum_{j=0}^{N} \frac{(a_0^*)^{N-j}}{\sqrt{(N-j)!}} \varphi_j$$

is a unitary operator with the inverse equal to U_N.

Step 1. We prove that U_N^* is a surjection, namely $U_N^* \mathcal{F}^{\leq N}(\mathscr{H}_+) = \mathscr{H}^{\otimes_s N}$. Let $\{u_n\}_{n=0}^{\infty}$ be an orthonormal basis for $\mathscr{H}$ and denote $a_n = a(u_n)$. Recall that $\mathcal{F}(\mathscr{H})$ has an orthonormal basis

$$(n_0! n_1! ...)^{-1/2} (a_0^*)^{n_0} (a_1^*)^{n_1} ... \Omega, \quad n_i = 0, 1, 2, ...$$

In particular, $\mathscr{H}^{\otimes_s N}$ has an orthonormal basis

$$(n_0! n_1! ...)^{-1/2} (a_0^*)^{n_0} (a_1^*)^{n_1} ... \Omega, \quad n_i = 0, 1, 2, ..., \sum_{i=0}^{\infty} n_i = N.$$

By the definition, $U_N^* \mathcal{F}^{\leq N}(\mathscr{H}_+)$ contains all these basis vectors, so $U_N^* \mathcal{F}^{\leq N}(\mathscr{H}_+) = \mathscr{H}^{\otimes_s N}$.

Step 2. We prove that $\|U_N^* \Phi\| = \|\Phi\|$ for any $\Phi = (\varphi_n)_{n=0}^{\infty} \in \mathcal{F}^{\leq N}(\mathscr{H}_+)$. By the definition,

$$\Psi := U_N^* \Phi = \sum_{j=0}^{N} \frac{(a_0^*)^{N-j}}{\sqrt{(N-j)!}} \varphi_j.$$

Since $\varphi_j \in \mathscr{H}_+^{\otimes_s j} \subset \mathscr{H}^{\otimes_s j}$, the vector $(a_0^*)^{N-j} \varphi_j$ belongs to $\mathscr{H}^{\otimes_s N}$. Thus $\Psi \in \mathscr{H}^{\otimes_s N}$.

Moreover, note that $a_0\varphi_j = 0$, and hence

$$a_0^m (a_0^*)^n \varphi_j = 0, \quad \text{if } m > n.$$

Thus the vectors $\{(a_0^*)^{N-j}\varphi_j\}_{j=0}^N$ are orthogonal. Moreover,

$$\begin{aligned}\|(a_0^*)^n \varphi_j\|^2 &= \langle (a_0^*)^{n-1}\varphi_j, (a_0 a_0^*)(a_0^*)^{n-1}\varphi_j\rangle \\ &= \langle (a_0^*)^{n-1}\varphi_j, (1 + a_0^* a_0)(a_0^*)^{n-1}\varphi_j\rangle \\ &= \langle (a_0^*)^{n-1}\varphi_j, n(a_0^*)^{n-1}\varphi_j\rangle \\ &= n\|(a_0^*)^{n-1}\varphi_j\|^2 = ... = n!\|\varphi_j\|^2.\end{aligned}$$

Consequently,

$$\|\Psi\|^2 = \sum_{j=0}^N \left\| \frac{(a_0^*)^{N-j}}{\sqrt{(N-j)!}}\varphi_j \right\|^2 = \sum_{j=0}^N \|\varphi_j\|^2.$$

Thus $\|U_N^*\Phi\| = \|\Phi\|$ for any $\Phi \in \mathcal{F}^{\leq N}(\mathscr{H}_+)$. Thus U_N^* is a unitary operator from $\mathcal{F}^{\leq N}(\mathscr{H}_+)$ to $\mathscr{H}^{\otimes_s N}$

Step 3. We prove that the inverse of U_N^* is exactly equal to U_N, namely if

$$\Psi := U_N^*\Phi = \sum_{j=0}^N \frac{(a_0^*)^{N-j}}{\sqrt{(N-j)!}}\varphi_j$$

then

$$Q^{\otimes i}\Big(\frac{a_0^{N-i}}{\sqrt{(N-i)!}}\Psi\Big) = \varphi_i, \quad \forall i = 0, 1, 2, ..., N.$$

We have

$$Q^{\otimes i}\Big(\frac{a_0^{N-i}}{\sqrt{(N-i)!}}\Psi\Big) = \sum_{j=0}^N \frac{Q^{\otimes i}}{\sqrt{(N-i)!}\sqrt{(N-j)!}} a_0^{N-i}(a_0^*)^{N-j}\varphi_j.$$

If $i < j$, then $N - i > N - j$, then $a_0^{N-i}(a_0^*)^{N-j}\varphi_j = 0$ because $a_0\varphi_j = 0$. If $i > j$, then $N-i < N-j$, then $a_0^{N-i}(a_0^*)^{N-j}\varphi_j$ is proportional to $(a_0^*)^{i-j}\varphi_j \in \mathscr{H}^{\otimes_s i}$, but $Q^{\otimes i}(a_0^*)^{i-j}\varphi_j = 0$ because $Qu_0 = 0$. Thus

$$Q^{\otimes i}\Big(\frac{a_0^{N-i}}{\sqrt{(N-i)!}}\Psi\Big) = \frac{Q^{\otimes i}}{(N-i)!} a_0^{N-i}(a_0^*)^{N-i}\varphi_i = \varphi_i.$$

Thus $U_N : \mathscr{H}^{\otimes_s N} \to \mathcal{F}^{\leq N}(\mathscr{H})$ defined before is the inverse of U_N^*.

Part II. Now we consider the action of $U_N(\cdot)U_N^*$. Let $\Phi = (\varphi_j)_{j=0}^\infty \in \mathcal{F}^{\leq N}(\mathscr{H}_+)$. Note that for any $f, g \in \mathscr{H}_+$, $a^*(f)a(g)$ does not change the total particle number, and more precisely it does not change the particle number in u_0 mode as well as the particle number in $\mathscr{H}_+$. Therefore,

$$\begin{aligned}
\Big\langle \Phi, U_N a^*(f)a(g)U_N^*\Phi \Big\rangle &= \Big\langle U_N^*\Phi, a^*(f)a(g)U_N^*\Phi \Big\rangle \\
&= \left\langle \sum_{i=0}^N \frac{(a_0^*)^{N-i}}{\sqrt{(N-i)!}}\varphi_i, a^*(f)a(g)\sum_{j=0}^N \frac{(a_0^*)^{N-j}}{\sqrt{(N-j)!}}\varphi_j \right\rangle \\
&= \sum_{j=0}^N \left\langle \frac{(a_0^*)^{N-j}}{\sqrt{(N-j)!}}\varphi_j, a^*(f)a(g)\frac{(a_0^*)^{N-j}}{\sqrt{(N-j)!}}\varphi_j \right\rangle \\
&= \sum_{j=0}^N \left\langle \varphi_j, a^*(f)a(g)\frac{a_0^{N-j}(a_0^*)^{N-j}}{(N-j)!}\varphi_j \right\rangle \\
&= \sum_{j=0}^N \langle \varphi_j, a^*(f)a(g)\varphi_j \rangle = \Big\langle \Phi, a^*(f)a(g)\Phi \Big\rangle.
\end{aligned}$$

By a similar computation, we also get

$$\Big\langle \Phi', U_N a^*(f)a(g)U_N^*\Phi \Big\rangle = \Big\langle \Phi', a^*(f)a(g)\Phi \Big\rangle, \quad \forall \Phi, \Phi' \in \mathcal{F}^{\leq N}(\mathscr{H}_+).$$

Thus we have the operator identity in $\mathcal{F}^{\leq N}(\mathscr{H}_+)$

$$U_N a^*(f)a(g)U_N^* = a^*(f)a(g), \quad \forall f, g \in \mathscr{H}_+.$$

Consequently, if we take an orthonormal basis $\{u_n\}_{n=0}^\infty$ for $\mathscr{H}$ and denote $a_n = a(u_n)$, then

$$U_N \mathcal{N}_+ U_N^* = U_N\Big(\sum_{n\geq 1}^\infty a_n^* a_n\Big)U_N^* = \mathcal{N}_+$$

which is equivalent to

$$U_N a_0^* a_0 U_N^* = U_N(N - \mathcal{N}_+)U_N^* = N - \mathcal{N}_+.$$

The remaining identity is left as an exercise. *q.e.d.*

Exercise. *Prove that for any* $f \in \mathscr{H}_+$ *we have the operator identity on* $\mathcal{F}^{\leq N}(\mathscr{H}_+)$

$$U_N a_0^* a(f) U_N^* = \sqrt{N - \mathcal{N}_+}\, a(f).$$

7.3 Transformed operator

Given the operator U_N, we can replace the heuristic approximation

$$H_N - Ne_{\mathrm{H}} \approx \mathbb{H}_{\mathrm{Bog}}.$$

by a better one

$$U_N(H_N - Ne_{\mathrm{H}})U_N^* \approx \mathbb{H}_{\mathrm{Bog}}$$

with two operators living in the same Hilbert space $\mathcal{F}(\mathscr{H}_+)$.

Let $\{u_n\}_{n=0}^\infty$ be an orthonormal basis for $\mathscr{H}$ and denote $a_n = a(u_n)$. We have the second quantization form

$$H_N = \sum_{m,n\geq 0} T_{mn} a_m^* a_n + \frac{1}{2(N-1)} \sum_{m,n,p,q\geq 0} W_{mnpq} a_m^* a_n^* a_p a_q$$

where

$$T_{mn} = \langle u_m, (-\Delta + V) u_n \rangle, \quad W_{mnpq} = \iint \overline{u_m(x) u_n(y)} w(x-y) u_p(x) u_q(y) \mathrm{d}x \mathrm{d}y.$$

Then from the above action of U_N, it is straightforward to compute $U_N(H_N - Ne_{\mathrm{H}})U_N^*$

Lemma (Transformed Hamiltonian)**.** *We have the operator identity on the truncated Fock space* $\mathcal{F}^{\leq N}(\mathscr{H}_+)$

$$U_N(H_N - Ne_{\mathrm{H}})U_N^* = \sum_{j=0}^4 A_j$$

where

$$A_0 = \frac{1}{2} W_{0000} \frac{\mathcal{N}_+(\mathcal{N}_+ - 1)}{N-1},$$

$$A_1 = \sum_{n\geq 1}\left(T_{0n} + W_{000n}\frac{N-\mathcal{N}_+-1}{N-1}\right)\sqrt{N-\mathcal{N}_+}a_n + h.c.,$$

$$A_2 = \sum_{m,n\geq 1}\langle u_m, (h+K)u_n\rangle a_m^* a_n + \sum_{m,n\geq 1}\langle u_m, \left(|u_0|^2 * w + K\right) u_n\rangle a_m^* a_n \frac{1-\mathcal{N}_+}{N-1}$$
$$+ \frac{1}{2}\sum_{m,n\geq 1}\left(\langle u_m, KJu_n\rangle a_n^* a_m^* \frac{\sqrt{(N-\mathcal{N}_+)(N-\mathcal{N}_+-1)}}{N-1} + h.c.\right),$$

$$A_3 = \frac{1}{N-1}\sum_{m,n,p\geq 1} W_{mnp0}a_m^* a_n^* a_p \sqrt{N-\mathcal{N}_+} + h.c.,$$

$$A_4 = \frac{1}{2(N-1)}\sum_{m,n,p,q\geq 1} W_{mnpq}a_m^* a_n^* a_p a_q.$$

This looks complicated, but if we formally take $N\to\infty$, then we see immediately that all A_0, A_1, A_3, A_4 are small ($o(1)$), while A_2 converges to the Bogoliubov transformation $\mathbb{H}_{\rm Bog}$. This will be justified rigorously later.

Proof of the theorem. The computation is tedious but straightforward, using the second quantization form and the action of U_N in the previous theorem.

For the kinetic terms:

- $T_{00}U_N a_0^* a_0 U_N^* = T_{00}(N-\mathcal{N}_+)$. The constant $T_{00}N$ is part of the Hartree energy $Ne_{\rm H}$. Recall that

  $$e_{\rm H} = \langle u_0, (-\Delta+V)u_0\rangle + \frac{1}{2}\iint |u_0(x)|^2 w(x-y)|u_0(y)|^2 {\rm d}x{\rm d}y = T_{00} + \frac{1}{2}W_{0000}.$$

  The other part $-T_{00}\mathcal{N}_+$ contributes to $-\mu\mathcal{N}_+$ in the first term the first term ${\rm d}\Gamma(h)$ of A_2. Recall that

  $$h = -\Delta + V + |u_0|^2 * w - \mu$$

  with

  $$\mu = \langle u_0, (-\Delta+V)u_0\rangle + \iint |u_0(x)|^2 w(x-y)|u_0(y)|^2 {\rm d}x{\rm d}y = T_{00} + W_{0000}.$$

- $T_{0n}U_N a_0^* a_n U_N^* = T_{0n}\sqrt{N-\mathcal{N}_+}a_n$ with $n\geq 1$. This term and its adjoint are part of A_1.

- $T_{mn}U_N a_m^* a_n U_N^* = T_{mn}a_m^* a_n$ with $m,n\geq 1$. This contributes to ${\rm d}\Gamma(h)$ of A_2.

For the interaction terms we have to use the CCR to rearrange creation/annihilation operators before applying the action of U_N (as we can only make sense for $U_N a^*(f)a(g)U_N^*$. Note that we always have the factor $(2(N-1))^{-1}W_{mnpq}$.

- $U_N a_0^* a_0^* a_0 a_0 U_N^* = U_N a_0^* a_0 (a_0^* a_0 - 1) U_N^* = (N - \mathcal{N}_+)(N-1-\mathcal{N}_+)$. The constant

$$\frac{1}{2(N-1)} W_{0000} N(N-1) = \frac{N}{2} W_{0000}$$

is part of the Hartree energy Ne_{H}. The term

$$\frac{1}{2(N-1)} W_{0000}(-2N-2)\mathcal{N}_+ = -W_{0000}\mathcal{N}_+$$

contributes to $-\mu\mathcal{N}_+$ in the first term $\mathrm{d}\Gamma(h)$ of A_2. The rest is A_0.

- $U_N a_0^* a_0^* a_0 a_n U_N^* = U_N a_0^* (a_0 a_0^* - 1) a_n U_N^* = (N - \mathcal{N}_+)\sqrt{N-\mathcal{N}_+}a_n - \sqrt{N-\mathcal{N}_+}a_n = (N-\mathcal{N}_+ - 1)\sqrt{N-\mathcal{N}_+}a_n$ with $n \geq 1$. Combining with the same contribution from $U_N a_0^* a_0^* a_n a_0 U_N^*$, we obtain

$$2 \times \frac{1}{2(N-1)} \sum_{n\geq 1} W_{000n}(N-\mathcal{N}_+ - 1)\sqrt{N-\mathcal{N}_+}a_n.$$

This term and its adjoints are part of A_1.

- $U_N a_0^* a_m^* a_0 a_n U_N^* = U_N a_0^* a_0 a_m^* a_n U_N^* = (N-\mathcal{N}_+)a_m^* a_n$ with $m, n \geq 1$. Combining with the same contribution from $U_N a_m^* a_0^* a_n a_0 U_N^*$ we obtain

$$2 \times \frac{1}{2(N-1)} \sum_{m,n\geq 1} W_{0m0n}(N-\mathcal{N}_+)a_m^* a_n = \sum_{m,n\geq 1} \langle u_m, (|u_0|^2 * w)u_n\rangle \frac{N-\mathcal{N}_+}{N-1} a_m^* a_n$$

which is part of A_2.

- $U_N a_0^* a_m^* a_n a_0 U_N^*$ and $U_N a_m^* a_0^* a_0 a_n U_N^*$ are also equal to $(N-\mathcal{N}_+)a_m^* a_n$ with $m, n \geq 1$, but they give

$$2 \times \frac{1}{2(N-1)} \sum_{m,n\geq 1} W_{0mn0}(N-\mathcal{N}_+)a_m^* a_n = \sum_{m,n\geq 1} \langle u_m, K u_n\rangle \frac{N-\mathcal{N}_+}{N-1} a_m^* a_n$$

which is another part of A_2.

- $U_N a_m^* a_n^* a_0 a_0 U_N^* = U_N (a_m^* a_0)(a_n^* a_0) U_N^* = a_m^* \sqrt{N-\mathcal{N}_+} a_n^* \sqrt{N-\mathcal{N}_+}$

$= a_m^* a_n^* \sqrt{N-\mathcal{N}_+}\sqrt{N-\mathcal{N}_+-1}$ with $m,n\geq 1$. This gives

$$\frac{1}{2(N-1)}\sum_{m,n\geq 1} W_{mn00} a_m^* a_n^* \sqrt{N-\mathcal{N}_+}\sqrt{N-\mathcal{N}_+-1}$$
$$=\sum_{m,n\geq 1}\frac{1}{2}\langle u_m, KJu_n\rangle a_m^* a_n^* \frac{\sqrt{(N-\mathcal{N}_+)(N-\mathcal{N}_+-1)}}{N-1}.$$

This term and its adjoint give us the last part of A_2.

- $U_N a_m^* a_n^* a_p a_0 U_N^* = U_N a_m^*(a_p a_n^* - \delta_{n=p}) a_0 U_N^* = U_N a_m^* a_p a_n^* a_0 U_N^* - \delta_{n=p} U_N a_m^* a_0 U_N^* = a_m^* a_p a_n^* \sqrt{N-\mathcal{N}_+} - \delta_{n=p} a_m^* \sqrt{N-\mathcal{N}_+} = a_m^* a_n^* a_p \sqrt{N-\mathcal{N}_+}$ with $m,n,p\geq 1$. Combining with the same contribution from $U_N a_m^* a_n^* a_0 a_p U_N^*$ we obtain

$$2\times\frac{1}{2(N-1)}\sum_{m,n,p\geq 1} W_{mnp0} a_m^* a_n^* a_p \sqrt{N-\mathcal{N}_+}.$$

  This term and its adjoint give us A_3.

- $U_N a_m^* a_n^* a_p a_q U_N^* = U_N a_m^*(a_p a_n^* - \delta_{n=p}) a_q U_N^* = U_N a_m^* a_p a_n^* a_q U_N^* - \delta_{n=p} U_N a_m^* a_q U_N^* = a_m^* a_p a_n^* a_q - \delta_{n=p} a_m^* a_q = a_m^* a_n^* a_p a_q$ with $m,n,p,q\geq 1$. We obtain

$$\frac{1}{2(N-1)}\sum_{m,n,p,q\geq 1} W_{mnpq} a_m^* a_n^* a_p a_q$$

  which gives us A_4.

This completes the computation of $U_N(H_N - Ne_{\rm H})U_N^*$. *q.e.d.*

7.4 Operator bounds on truncated Fock space

Now we compare the transformed operator $U_N(H_N - Ne_{\rm H})U_N^*$ and the Bogoliubov Hamiltonian $\mathbb{H}_{\rm Bog}$.

Lemma. *Let* $\mathbb{1}^{\leq N} := \mathbb{1}(\mathcal{N}_+ \leq N)$. *Then*

$$\pm \mathbb{1}^{\leq N}\Big(U_N(H_N - Ne_{\rm H})U_N^* - \mathbb{H}_{\rm Bog}\Big)\mathbb{1}^{\leq N} \leq C(N^{-1/2}\mathcal{N}_+^2 + N^{-1}).$$

Note that $\mathbb{H}_{\rm Bog}$ acts on $\mathcal{F}(\mathscr{H}_+)$, so the particle number cut-off $\mathbb{1}^{\leq N} := \mathbb{1}(\mathcal{N}_+ \leq N)$. is necessary to project it to the truncated Fock space $\mathcal{F}^{\leq N}(\mathscr{H}_+)$. Putting differently, the bound in the lemma is equivalent to

$$\langle \Phi, \Big(U_N(H_N - Ne_{\rm H})U_N^* - \mathbb{H}_{\rm Bog} \Big) \Phi \rangle \le C \langle \Phi, (N^{-1/2}\mathcal{N}_+^2 + N^{-1})\Phi \rangle, \quad \forall \Phi \in \mathcal{F}^{\le N}(\mathscr{H}_+).$$

Proof. For simplicity of notation we will often not write the projection $\mathbb{1}^{\le N}$ and think of quadratic form estimates on $\mathcal{F}^{\le N}(\mathscr{H}_+)$ instead. From the previous computation, we have

$$U_N(H_N - Ne_{\rm H})U_N^* = \sum_{j=0}^{4} A_j.$$

We will estimate term by term.

Estimate A_0. We have

$$0 \le A_0 = \frac{1}{2} W_{0000} \frac{\mathcal{N}_+(\mathcal{N}_+ - 1)}{N-1} \le C \frac{\mathcal{N}_+^2}{N}.$$

Estimate A_1. Using Hartree equation $hu_0 = 0$ we have

$$0 = \langle hu_0, u_n \rangle = \langle u_0, (-\Delta + V + |u_0|^2 * w - \mu) u_n \rangle = T_{0n} + W_{000n}.$$

Therefore,

$$\begin{aligned} A_1 &= \sum_{n\ge 1} \left(T_{0n} + W_{000n} \frac{N - \mathcal{N}_+ - 1}{N-1} \right) \sqrt{N - \mathcal{N}_+}\, a_n + h.c. \\ &= - \sum_{n \ge 1} W_{000n} \frac{\mathcal{N}_+}{N-1} \sqrt{N - \mathcal{N}_+}\, a_n + h.c. \end{aligned}$$

By the Cauchy-Schwarz inequality,

$$\begin{aligned} \pm A_1 &\le \sum_{n\ge 1} \left(\varepsilon^{-1} |W_{000n}|^2 \Big(\frac{\mathcal{N}_+}{N-1} \Big) (N - \mathcal{N}_+) \Big(\frac{\mathcal{N}_+}{N-1} \Big) + \varepsilon a_n^* a_n \right) \\ &\le C\varepsilon^{-1} \frac{\mathcal{N}_+^2 (N - \mathcal{N}_+)}{(N-1)^2} + \varepsilon \mathcal{N}_+ \le C \varepsilon^{-1} \frac{\mathcal{N}_+^2}{N} + \varepsilon \mathcal{N}_+, \quad \forall \varepsilon > 0. \end{aligned}$$

Here we have used

$$\sum_{n\ge 1} |W_{000n}|^2 = \sum_{n \ge 1} |\langle u_0, K u_n \rangle|^2 \le \|K\|_{\rm HS}^2 < \infty.$$

Choosing $\varepsilon = N^{-1/2}$ we obtain

$$\pm A_1 \le C N^{-1/2} \mathcal{N}_+^2.$$

Estimate A_2**.** We have

$$\begin{aligned} A_2 &= \sum_{m,n\ge 1} \langle u_m, (h+K)u_n\rangle\, a_m^* a_n + \sum_{m,n\ge 1} \left\langle u_m, \left(|u_0|^2 * w + K\right) u_n\right\rangle a_m^* a_n \frac{1-\mathcal{N}_+}{N-1} \\ &+ \frac{1}{2}\sum_{m,n\ge 1}\left(\langle u_m, KJu_n\rangle a_m^* a_n^* \frac{\sqrt{(N-\mathcal{N}_+)(N-\mathcal{N}_+-1)}}{N-1} + h.c.\right) \\ &= \mathbb{H}_{\rm Bog} + \sum_{m,n\ge 1} \left\langle u_m, \left(|u_0|^2 * w + K\right) u_n\right\rangle a_m^* a_n \frac{1-\mathcal{N}_+}{N-1} + \frac{1}{2}(B^* X + XB) \end{aligned}$$

where

$$B^* := \sum_{m,n\ge 1} \langle u_m, KJu_n\rangle a_m^* a_n^*, \quad X := \frac{\sqrt{(N-\mathcal{N}_+)(N-\mathcal{N}_+-1)}}{N-1} - 1.$$

We have

$$\pm \sum_{m,n\ge 1} \left\langle u_m, \left(|u_0|^2 * w + K\right) u_n\right\rangle a_m^* a_n = \pm {\rm d}\Gamma(Q(|u_0|^2 * w + K)Q) \le {\rm d}\Gamma(QCQ) = C\mathcal{N}_+.$$

Moreover, the relevant operator commutes with $\mathcal{N}_+$. Therefore,

$$\pm \sum_{m,n\ge 1} \left\langle u_m, \left(|u_0|^2 * w + K\right) u_n\right\rangle a_m^* a_n \frac{1-\mathcal{N}_+}{N-1} \le C\frac{\mathcal{N}_+^2}{N}.$$

On the other hand, by the Cauchy-Schwarz inequality

$$\pm \frac{1}{2}(B^* X + XB) \le \frac{1}{2}(\varepsilon B^* B + \varepsilon^{-1} X^2), \quad \forall \varepsilon > 0.$$

It is straightforward to see that

$$\begin{aligned} X^2 &= \left| \frac{\sqrt{(N-\mathcal{N}_+)(N-\mathcal{N}_+-1)}}{N-1} - 1\right|^2 = \left| \sqrt{\left(1-\frac{\mathcal{N}_+-1}{N-1}\right)\left(1-\frac{\mathcal{N}_+}{N-1}\right)} - 1\right|^2 \\ &\le \left| \left(1-\frac{\mathcal{N}_+-1}{N-1}\right)\left(1-\frac{\mathcal{N}_+}{N-1}\right) - 1\right|^2 \le \frac{C(\mathcal{N}_++1)^2}{N^2} \end{aligned}$$

Exercise. *Let K be a Hilbert-Schmidt operator on a Hilbert space $\mathscr{H}$. Let $\{u_n\}_{n\geq 1}$ be an orthonormal family of $\mathscr{H}$. Consider*

$$B^* := \sum_{m,n\geq 1} \langle u_m, KJu_n\rangle a_m^* a_n^*.$$

Prove that

$$B^*B \leq \|K\|_{\mathrm{HS}}^2 \mathcal{N}^2.$$

Thus

$$\pm\frac{1}{2}(B^*X + XB) \leq \frac{1}{2}(\varepsilon B^*B + \varepsilon^{-1}X^2) \leq C\varepsilon\mathcal{N}_+^2 + C_\varepsilon^{-1}\frac{C(\mathcal{N}_+ + 1)^2}{N^2}.$$

By choosing $\varepsilon = N^{-1}$ we conclude that

$$\pm\frac{1}{2}(B^*X + XB) \leq C\frac{(\mathcal{N}_+ + 1)^2}{N}$$

Thus in summary,

$$\pm(A_2 - \mathbb{H}_{\mathrm{Bog}}) \leq C\frac{(\mathcal{N}_+ + 1)^2}{N}.$$

Estimate A_4. Consider

$$\begin{aligned} A_4 &= \frac{1}{2(N-1)} \sum_{m,n,p,q\geq 1} W_{mnpq} a_m^* a_n^* a_p a_q \\ &= \frac{1}{2(N-1)} \sum_{m,n,p,q\geq 0} \langle u_m \otimes u_n, (Q\otimes QwQ\otimes Q)u_p \otimes u_q\rangle a_m^* a_n^* a_p a_q \end{aligned}$$

Thus A_4 is the second quantization of the two-body operator $(N-1)^{-1}Q\otimes QwQ\otimes Q$ (here $w = w(x-y)$ is the multiplication operator). Since w is bounded, we have

$$\pm Q\otimes QwQ\otimes Q \leq \|w\|_{L^\infty} Q\otimes Q.$$

Therefore, in the second quantization form we have

$$\pm A_4 \leq \frac{\|w\|_{L^\infty}}{2(N-1)}\mathcal{N}_+(\mathcal{N}_+ - 1) \leq \frac{C\mathcal{N}_+^2}{N}.$$

Estimate A_3. Finally, we consider

$$\begin{aligned} A_3 &= \frac{1}{N-1}\sum_{m,n,p\geq 1} W_{mnp0} a_m^* a_n^* a_p \sqrt{N-\mathcal{N}_+} + h.c. \\ &= \frac{1}{N-1} U_N \Big(\sum_{m,n,p\geq 1} W_{mnp0} a_m^* a_n^* a_p a_0 + h.c. \Big) U_N^* \\ &= \frac{1}{N-1} U_N \Big(\sum_{m,n,p,q\geq 0} \langle u_m \otimes u_n, (Q\otimes QwQ\otimes P) u_p \otimes u_q \rangle a_m^* a_n^* a_p a_q + h.c. \Big) U_N^* \end{aligned}$$

Thus up to a transformation by U_N, A_3 is the second quantization of the two-body operator

$$(N-1)^{-1}\Big(Q\otimes QwQ\otimes P + Q\otimes QwP\otimes Q + h.c.\Big).$$

By the Cauchy-Schwarz inequality, we have the two-body inequalities

$$\begin{aligned} &\pm \Big(Q\otimes QwQ\otimes P + Q\otimes QwP\otimes Q + h.c.\Big) \\ &\leq 2\varepsilon^{-1} Q\otimes Q|w|Q\otimes Q + \varepsilon Q\otimes P|w|Q\otimes P + \varepsilon P\otimes Q|w|P\otimes Q, \\ &\leq \|w\|_{L^\infty}\Big(2\varepsilon^{-1} Q\otimes Q + \varepsilon P\otimes Q + \varepsilon Q\otimes P\Big), \quad \forall \varepsilon > 0. \end{aligned}$$

In the second quantization form, we obtain

$$\pm \sum_{m,n,p,q\geq 0} \langle u_m \otimes u_n, (Q\otimes QwQ\otimes P) u_p \otimes u_q \rangle a_m^* a_n^* a_p a_q + h.c. \leq C(\varepsilon^{-1}\mathcal{N}_+^2 + \varepsilon(N-\mathcal{N}_+)\mathcal{N}_+).$$

Thus

$$\pm A_3 \leq \frac{C}{N-1} U_N \Big(\varepsilon^{-1}\mathcal{N}_+^2 + \varepsilon N \mathcal{N}_+\Big) U_N^* \leq C\Big(\varepsilon^{-1}\frac{\mathcal{N}_+^2}{N} + \varepsilon \mathcal{N}_+\Big).$$

Choosing $\varepsilon = N^{-1/2}$ we get

$$\pm A_3 \leq C N^{-1/2} \mathcal{N}_+^2.$$

Thus in summary, we have prove that

$$\pm\Big(U_N(H_N - N e_{\mathrm{H}})U_N^* - \mathbb{H}_{\mathrm{Bog}}\Big) \leq C N^{-1/2}\mathcal{N}_+^2 + C N^{-1}$$

as a quadratic form estimate on $\mathcal{F}^{\leq N}(\mathscr{H}_+)$. This completes the proof of the lemma. *q.e.d.*

7.5 Improved condensation

Recall that under the condition $0 \le \widehat{w} \in L^1(\mathbb{R}^d)$ for any wave function $\Psi \in \mathscr{H}^{\otimes_s N}$ satisfying $\langle \Psi, H_N \Psi \rangle \le N e_{\mathrm{H}} + \mathcal{O}(1)$ we have the complete BEC on the Hartree minimizer u_0:

$$\langle \Psi, \mathcal{N}_+ \Psi \rangle \le \mathcal{O}(1)$$

where $\mathcal{N}_+ = \mathrm{d}\Gamma(Q)$ with $Q = 1 - |u_0\rangle\langle u_0|$. Since $U_N \mathcal{N}_+ U_N^* = \mathcal{N}_+$, the same bound holds if Ψ replaced by $U_N \Psi$.

From the previous section, to control the error of $U_N(H_N - N e_{\mathrm{H}})U_N^* - \mathbb{H}_{\mathrm{Bog}}$, it is desirable to have an upper bound on $\langle \Psi_N, \mathcal{N}_+^2 \Psi_N \rangle$. This improved condensation is proved in this section.

Lemma. *Assume that $0 \le \widehat{w} \in L^1(\mathbb{R}^d)$. Let $\Psi \in \mathscr{H}^{\otimes_s N}$ be an eigenfunction of H_N with an eigenvalue $\mu_n(H_N) = N e_{\mathrm{H}} + \mathcal{O}(1)$. Then*

$$\langle \Psi, \mathcal{N}_+^2 \Psi \rangle \le \mathcal{O}(1).$$

Actually, the proof below can be extended to show that $\langle \Psi, \mathcal{N}_+^k \Psi \rangle \le \mathcal{O}_k(1)$ for all $k \ge 1$. However, the case $k = 2$ is sufficient for our application.

Proof. **Step 1.** From the Schrödinger equation $H_N \Psi = \mu_n \Psi$ we have

$$\begin{aligned} 0 &= \langle \Psi, \Big[\mathcal{N}_+^2 (H_N - \mu_n) + (H_N - \mu_n)\mathcal{N}_+^2\Big] \Psi \rangle \\ &= 2\langle \Psi, \mathcal{N}_+ (H_N - \mu_n) \mathcal{N}_+ \Psi \rangle + \langle \Psi, [[H_N, \mathcal{N}_+], \mathcal{N}_+] \Psi \rangle. \end{aligned}$$

Here we used the formula of "double commutator" (for any operators A, X)

$$[[A, X], X] = (AX - XA)X - X(AX - XA) = AX^2 + X^2 A - 2XAX.$$

From the proof of the complete BEC, we have

$$H_N - \mu_n \ge H_N - N e_{\mathrm{H}} - C \ge c_0 \mathcal{N}_+ - C$$

for some constants $c_0 > 0$. Therefore,

$$2\mathcal{N}_+ (H_N - E_N) \mathcal{N}_+ \ge 2 c_0 \mathcal{N}_+^3 - C \mathcal{N}_+^2 \ge c_0 \mathcal{N}_+^3 - C.$$

Thus

$$2\langle\Psi, \mathcal{N}_+(H_N - E_N)\mathcal{N}_+\Psi\rangle \geq c_0\langle\Psi, \mathcal{N}_+^3\Psi\rangle - C.$$

It remains to bound the double commutator $\langle\Psi, [[H_N, \mathcal{N}_+], \mathcal{N}_+]\Psi\rangle$.

Step 2. We compute $[H_N, \mathcal{N}_+]$. We use

$$\mathcal{N}_+ = \sum_{n\geq 1} a_n^* a_n$$

and the second quantization form

$$H_N = \sum_{m,n\geq 0} T_{mn} a_m^* a_n + \frac{1}{2(N-1)} \sum_{m,n,p,q\geq 0} W_{mnpq} a_m^* a_n^* a_p a_q$$

where

$$T_{mn} = \langle u_m, (-\Delta + V)u_n\rangle, \quad W_{mnpq} = \iint \overline{u_m(x)u_n(y)} w(x-y) u_p(x) u_q(y) \mathrm{d}x\mathrm{d}y.$$

Since

$$[a_m^*, a_\ell^* a_\ell] = a_\ell^*[a_m^*, a_\ell] = -\delta_{m=\ell} a_m^*, \quad [a_n, a_\ell^* a_\ell] = \delta_{n=\ell} a_n.$$

we can compute

$$[a_m^* a_n, a_\ell^* a_\ell] = [a_m^*, a_\ell^* a_\ell] a_n + a_m^*[a_n, a_\ell^* a_\ell] = (\delta_{n=\ell} - \delta_{m=\ell}) a_m^* a_n.$$

Therefore,

$$\begin{aligned}
\sum_{m,n\geq 0} T_{mn}[a_m^* a_n, \mathcal{N}_+] &= \sum_{m,n\geq 0} \sum_{\ell\geq 1} T_{mn}[a_m^* a_n, a_\ell^* a_\ell] \\
&= \sum_{m,n\geq 0} \sum_{\ell\geq 1} (\delta_{n=\ell} - \delta_{m=\ell}) T_{mn} a_m^* a_n \\
&= \sum_{n\geq 1} (T_{0n} a_0^* a_n - h.c.).
\end{aligned}$$

Here we have used the simplification

$$\sum_{\ell\geq 1} (\delta_{n=\ell} - \delta_{m=\ell}) = \sum_{\ell\geq 1} \delta_{n=\ell} - \sum_{\ell\geq 1} \delta_{m=\ell} = \mathbb{1}(n\geq 1) - \mathbb{1}(m\geq 1)$$

$$= \begin{cases} 0 & \text{if } m = n = 0 \text{ or } m, n \geq 1 \\ 1 & \text{if } n \neq m = 0 \\ -1 & \text{if } m \neq n = 0. \end{cases}$$

Similarly,

$$\begin{aligned}[][a_m^* a_n^* a_p a_q, a_\ell^* a_\ell] &= [a_m^*, a_\ell^* a_\ell] a_n^* a_p a_q + a_m^* [a_n^*, a_\ell^* a_\ell] a_p a_q + a_m^* a_n^* [a_p, a_\ell^* a_\ell] a_q + a_m^* a_n^* a_p [a_q, a_\ell^* a_\ell] \\ &= \Big(\delta_{p=\ell} + \delta_{q=\ell} - \delta_{m=\ell} - \delta_{n=\ell} \Big) a_m^* a_n^* a_p a_q \end{aligned}$$

Thus

$$\begin{aligned} &\frac{1}{2(N-1)} \sum_{m,n,p,q \geq 0} W_{m,n,p,q} [a_m^* a_n^* a_p a_q, \mathcal{N}_+] \\ &= \frac{1}{2(N-1)} \sum_{m,n,p,q \geq 0} W_{m,n,p,q} \sum_{\ell \geq 1} [a_m^* a_n^* a_p a_q, a_\ell^* a_\ell] \\ &= \frac{1}{2(N-1)} \sum_{m,n,p,q \geq 0} \sum_{\ell \geq 1} \Big(\delta_{p=\ell} + \delta_{q=\ell} - \delta_{m=\ell} - \delta_{n=\ell} \Big) W_{mnpq} a_m^* a_n^* a_p a_q \\ &= \frac{1}{2(N-1)} \sum_{m,n,p,q \geq 0} \Big(\mathbb{1}(p \geq 1) + \mathbb{1}(q \geq 1) - \mathbb{1}(m \geq 1) - \mathbb{1}(n \geq 1) \Big) W_{mnpq} a_m^* a_n^* a_p a_q \\ &= \frac{1}{N-1} \sum_{n \geq 1} (W_{000n} a_0^* a_0^* a_0 a_n - h.c.) \\ &+ \frac{1}{N-1} \sum_{m,n \geq 1} (W_{00mn} a_0^* a_0^* a_m a_n - h.c.) \\ &+ \frac{1}{N-1} \sum_{m,n,p \geq 1} (W_{0mnp} a_0^* a_m^* a_n a_p - h.c.). \end{aligned}$$

In summary,

$$\begin{aligned}[][H_N, \mathcal{N}_+] = \sum_{n \geq 1} (T_{0n} a_0^* a_n - h.c.). + \frac{1}{N-1} \sum_{n \geq 1} (W_{000n} a_0^* a_0^* a_0 a_n - h.c.) \\ + \frac{1}{N-1} \sum_{m,n \geq 1} (W_{00mn} a_0^* a_0^* a_m a_n - h.c.) + \frac{1}{N-1} \sum_{m,n,p \geq 1} (W_{0mnp} a_0^* a_m^* a_n a_p - h.c.). \end{aligned}$$

Recall that by Hartree equation

$$T_{0n} + W_{000n} = \langle u_0, (-\Delta + V + |u_0|^2 * w) u_n \rangle = \langle u_0, (h + \mu) u_n \rangle = 0, \quad \forall n \geq 1.$$

Therefore,

$$\begin{aligned}
&\sum_{n\geq 1} T_{0n} a_0^* a_n + \frac{1}{N-1}\sum_{n\geq 1} W_{000n} a_0^* a_0^* a_0 a_n \\
&= \frac{1}{N-1}\sum_{n\geq 1} W_{000n}(-(N-1)a_0^* a_n + a_0^* a_n(N-\mathcal{N}_+)) \\
&= -\frac{1}{N-1}\sum_{n\geq 1} W_{000n}(a_0^* a_n(\mathcal{N}_+ - 1)) = -\frac{1}{N-1}\sum_{n\geq 1} W_{000n}(a_0^*\mathcal{N}_+ a_n)
\end{aligned}$$

Thus

$$\begin{aligned}
[H_N, \mathcal{N}_+] = &-\frac{1}{N-1}\sum_{n\geq 1}(W_{000n} a_0^*\mathcal{N}_+ a_n - h.c.) \\
&+ \frac{1}{N-1}\sum_{m,n\geq 1}(W_{00mn} a_0^* a_0^* a_m a_n - h.c.) + \frac{1}{N-1}\sum_{m,n,p\geq 1}(W_{0mnp} a_0^* a_m^* a_n a_p - h.c.).
\end{aligned}$$

Step 3. We compute $[[H_N, \mathcal{N}_+], \mathcal{N}_+]$. Note that

$$[A - A^*, \mathcal{N}_+] = [A, \mathcal{N}_+] - [A^*, \mathcal{N}_+] = [A, \mathcal{N}_+] + h.c.$$

Therefore,

$$\begin{aligned}
[[H_N, \mathcal{N}_+], \mathcal{N}_+] = &-\frac{1}{N-1}\sum_{n\geq 1}(W_{000n}[a_0^*\mathcal{N}_+ a_n, \mathcal{N}_+] + h.c.) \\
&+ \frac{1}{N-1}\sum_{m,n\geq 1}(W_{00mn}[a_0^* a_0^* a_m a_n, \mathcal{N}_+] + h.c.) \\
&+ \frac{1}{N-1}\sum_{m,n,p\geq 1}(W_{0mnp}[a_0^* a_m^* a_n a_p, \mathcal{N}_+] + h.c.).
\end{aligned}$$

Using

$$\begin{aligned}
[a_n, \mathcal{N}_+] &= a_n\mathcal{N}_+ - \mathcal{N}_+ a_n = (\mathcal{N}_+ + 1)a_n - \mathcal{N}_+ a_n = a_n, \quad \forall n \geq 1, \\
[a_m a_n, \mathcal{N}_+] &= a_m a_n \mathcal{N}_+ - \mathcal{N}_+ a_m a_n = 2a_m a_n, \quad \forall m, n \geq 1, \\
[a_m^* a_n a_p, \mathcal{N}_+] &= a_m^* a_n a_p \mathcal{N}_+ - \mathcal{N}_+ a_m^* a_n a_p = a_m^* a_n a_p, \quad \forall m, n, p \geq 1
\end{aligned}$$

we obtain

$$
\begin{aligned}
[[H_N, \mathcal{N}_+], \mathcal{N}_+] = &-\frac{1}{N-1}\sum_{n\geq 1}(W_{000n}a_0^*\mathcal{N}_+ a_n + h.c.) \\
&+ \frac{2}{N-1}\sum_{m,n\geq 1}(W_{00mn}a_0^*a_0^*a_m a_n + h.c.) \\
&+ \frac{1}{N-1}\sum_{m,n,p\geq 1}(W_{0mnp}a_0^*a_m^*a_n a_p + h.c.).
\end{aligned}
$$

Step 4. Now we estimate $\langle \Psi, [[H_N, \mathcal{N}_+]\mathcal{N}_+]\Psi\rangle$. From the above computation we have

$$\langle \Psi, [[H_N, \mathcal{N}_+], \mathcal{N}_+]\Psi\rangle = I_1 + I_2 + I_3$$

where

$$
\begin{aligned}
I_1 &= -2\Re\frac{1}{N-1}\sum_{n\geq 1} W_{000n}\langle \Psi, a_0^*\mathcal{N}_+ a_n\Psi\rangle, \\
I_2 &= 4\Re\frac{1}{N-1}\sum_{m,n\geq 1} W_{00mn}\langle \Psi, a_0^*a_0^*a_m a_n\Psi\rangle, \\
I_3 &= 2\Re\frac{1}{N-1}\sum_{m,n,p\geq 1} W_{0mnp}\langle \Psi, a_0^*a_m^*a_n a_p\Psi\rangle.
\end{aligned}
$$

We bound term by term.

Estimate I_1. By the Cauchy-Schwarz inequality, we have

$$
\begin{aligned}
|I_1| &\leq 2\frac{1}{N-1}\sum_{n\geq 1}|W_{000n}||\langle \Psi, a_0^*\mathcal{N}_+ a_n\Psi\rangle| \\
&\leq \frac{C}{N}\sum_{n\geq 1}|W_{000n}|\|\mathcal{N}_+ a_0\Psi\|\|a_n\Psi\| \\
&\leq \frac{C}{N}\|\mathcal{N}_+ a_0\Psi\|\sqrt{\sum_{n\geq 1}|W_{000n}|^2}\sqrt{\sum_{n\geq 1}\|a_n\Psi\|^2} \\
&\leq \frac{C}{N}\sqrt{\langle \Psi, a_0^*\mathcal{N}_+^2 a_0\Psi\rangle}\sqrt{\sum_{n\geq 1}\langle \Psi, a_n^*a_n\Psi\rangle} \\
&\leq \frac{C}{N}\sqrt{\langle \Psi, \mathcal{N}_+^2 N\Psi\rangle}\sqrt{\langle \Psi, \mathcal{N}_+\Psi\rangle} \\
&\leq \frac{C}{\sqrt{N}}\langle \Psi, \mathcal{N}_+^2\Psi\rangle.
\end{aligned}
$$

Here recall that $W_{000n} = \langle u_0, K u_n \rangle$ with $K(x,y) = u_0(x)w(x-y)u_0(y)$.

Estimate I_2. By the Cauchy-Schwarz inequality, we have

$$\begin{aligned}
|I_2| &\le 4\frac{1}{N-1}\sum_{m,n\ge 1} |W_{00mn}||\langle \Psi, a_0^* a_0^* a_m a_n \Psi\rangle| \\
&\le \frac{C}{N}\sum_{m,n\ge 1} |W_{00mn}|\|a_0 a_0 \Psi\|\|a_m a_n \Psi\| \\
&\le \frac{C}{N}\|a_0 a_0\Psi\|\sqrt{\sum_{m,n\ge 1}|W_{00mn}|^2}\sqrt{\sum_{m,n\ge 1}\|a_m a_n \Psi\|^2} \\
&\le \frac{C}{N}\sqrt{\langle \Psi, a_0^* a_0^* a_0 a_0 \Psi\rangle}\sqrt{\sum_{m,n\ge 1}\langle \Psi, a_m^* a_n^* a_m a_n \Psi\rangle} \\
&\le \frac{C}{N}\sqrt{\langle \Psi, N^2 \Psi\rangle}\sqrt{\langle \Psi, \mathcal{N}_+^2 \Psi\rangle} = C\langle \Psi, (\mathcal{N}_+ + 1)^2 \Psi\rangle.
\end{aligned}$$

Here recall that $W_{00mn} = \overline{\langle u_m, KJu_n\rangle}$ with $K(x,y) = u_0(x)w(x-y)u_0(y)$.

Estimate I_3. Recall that from the analysis of A_3 in the previous section, we have the quadratic form estimate

$$\begin{aligned}
&\pm\frac{1}{N-1}\Big(\sum_{m,n,p\ge 1}(W_{0mnp}a_0^* a_m^* a_n a_p + h.c.) \\
&= \pm\frac{1}{N-1}\Big(\sum_{m,n,p,q\ge 0}\langle u_m\otimes u_n, (P\otimes QwQ\otimes Q)u_p\otimes u_q\rangle a_m^* a_n^* a_p a_q + h.c.\Big) \\
&\le \frac{C}{N}\Big(\varepsilon^{-1}\mathcal{N}_+^2 + \varepsilon N\mathcal{N}_+\Big) \le \frac{C}{\sqrt{N}}\mathcal{N}_+^2.
\end{aligned}$$

(Here we took $\varepsilon = N^{-1/2}$.) Thus

$$\pm I_3 \le \frac{C}{\sqrt{N}}\langle \Psi, \mathcal{N}_+^2 \Psi\rangle.$$

In summary, we have

$$\pm\langle \Psi, [[H_N, \mathcal{N}_+], \mathcal{N}_+]\Psi\rangle = \pm(I_1 + I_2 + I_3) \le C\langle \Psi, (\mathcal{N}_+ + 1)^2\Psi\rangle$$

Step 5: Conclusion. We have

$$\begin{aligned}
0 &= 2\langle \Psi, \mathcal{N}_+(H_N - E_N)\mathcal{N}_+\Psi\rangle + \langle \Psi, [[H_N, \mathcal{N}_+], \mathcal{N}_+]\Psi\rangle \\
&\ge c_0\langle \Psi, \mathcal{N}_+^3\Psi\rangle - C - C\langle \Psi, (\mathcal{N}_+ + 1)^2\Psi\rangle.
\end{aligned}$$

This implies that

$$\langle \Psi, \mathcal{N}_+^3 \Psi \rangle \le C.$$

Consequently,

$$\langle \Psi, \mathcal{N}_+^2 \Psi \rangle \le C.$$

q.e.d.

We can prove $\langle \Phi, \mathcal{N}_+^2 \Phi \rangle < \infty$ for eigenfunctions of the Bogoliubov Hamiltonian, using either the above strategy or the fact that $\mathbb{H}_{\rm Bog}$ can be diagonalized by a Bogoliubov transformation. More gerenaly, we have

Exercise. *Let $\Phi \in \mathcal{F}(\mathscr{H}_+)$ be an eigenfunction of the Bogoliubov Hamiltonian $\mathbb{H}_{\rm Bog}$. Prove that*

$$\langle \Phi, \mathcal{N}_+^k \Phi \rangle < \infty, \quad \forall k \ge 1.$$

7.6 Derivation of Bogoliubov excitation spectrum

Now we are able to rigorously justify Bogoliubov approximation. Recall that we are considering the Hamiltonian

$$H_N = \sum_{i=1}^N (-\Delta_{x_i} + V(x_i)) + \frac{1}{N-1} \sum_{1 \le i < j \le N} w(x_i - x_j)$$

acting on $\mathscr{H}^{\otimes_s N}$, $\mathscr{H} = L^2(\mathbb{R}^d)$. The condensate is described by Hartree minimizer u_0. The result below says that the particles outside the condensation is effectively described by the Bogoliubov Hamiltonian

$$\mathbb{H}_{\rm Bog} = \sum_{m,n \ge 1} \langle u_m, (h+K) u_n \rangle a_m^* a_n + \frac{1}{2} \sum_{m,n \ge 1} \Big(\langle u_m, K J u_n \rangle a_m^* a_n^* + h.c. \Big)$$

on the excited Fock space $\mathcal{F}(\mathscr{H}_+)$ where

$$h = -\Delta + V + |u_0|^2 * w - \mu, \quad K(x,y) = u_0(x) w(x-y) u_0(y).$$

Theorem. *Assume that*

- *Trapping potential:* $V \in L^\infty_{\mathrm{loc}}(\mathbb{R}^d, \mathbb{R})$, $\lim_{|x|\to\infty} V(x) = +\infty$;
- *Positive-type bounded interaction:* $0 \le \widehat{w} \in L^1(\mathbb{R}^d)$.

Then the following statements hold true.

- **Convergence of eigenvalues.** *For any* $i = 1, 2, ...$, *the* i*-th eigenvalue of* H_N *satisfies*
$$\lim_{N\to\infty} \Big(\mu_i(H_N) - Ne_{\mathrm{H}} - \mu_i(\mathbb{H}_{\mathrm{Bog}}) \Big) = 0.$$
- **Convergence of eigenstates.** *Let* $\Psi_N^{(i)}$ *be an eigenfunction of* H_N *with the* i*-th eigenvalue* $\mu_i(H_N)$*. Then up to a subsequence as* $N \to \infty$*, we have*
$$\lim_{N\to\infty} U_N \Psi_N^{(i)} = \Phi^{(i)}$$
strongly in $\mathcal{F}(\mathscr{H}_+)$*, where* $\Phi^{(i)}$ *is an eigenfunction of* $\mathbb{H}_{\mathrm{Bog}}$ *with the* i*-th eigenvalue* $\mu_i(\mathbb{H}_{\mathrm{Bog}})$.

Remark: When $n = 1$, the ground state $\Phi^{(1)}$ of $\mathbb{H}_{\mathrm{Bog}}$ is unique (up to a phase), and hence, up to a correct choice of the phase, we have the convergence for the whole sequence $N \to \infty$. More precisely, we can find a sequence of complex numbers $\{z_N\}$, $|z_N| = 1$ such that

$$\lim_{N\to\infty} z_N U_N \Psi_N^{(1)} = \Phi^{(1)}.$$

Proof. To make the idea transparent, let us consider the ground state first, and then explain the extension for higher eigenvalues.

Step 1: Ground state energy - lower bound. Let $\Psi_N^{(1)} \in \mathscr{H}^{\otimes_s N}$ be a ground state for H_N. By the validity of Hartree theory we know that

$$\langle \Psi_N^{(1)}, H_N \Psi_N^{(1)} \rangle = \mu_1(H_N) = E_N = Ne_{\mathrm{H}} + \mathcal{O}(1).$$

Therefore, we have the (improved) condensation

$$\langle \Psi_N^{(1)}, \mathcal{N}_+^2 \Psi_N^{(1)} \rangle = \langle U_N \Psi_N^{(1)}, \mathcal{N}_+^2 U_N \Psi_N^{(1)} \rangle = \mathcal{O}(1).$$

On the other hand, we have the operator bound on $\mathcal{F}^{\leq N}(\mathscr{H}_+)$

$$\pm \mathbb{1}^{\leq N}\Big(U_N(H_N - Ne_{\rm H})U_N^* - \mathbb{H}_{\rm Bog}\Big)\mathbb{1}^{\leq N} \leq CN^{-1/2}(\mathcal{N}_+^2 + 1).$$

Here recall that $\mathbb{1}^{\leq N} = \mathbb{1}(\mathcal{N}_+ \leq N)$ is the projection on the truncated Fock space $\mathcal{F}^{\leq N}(\mathscr{H}_+)$. Taking the expectation against $U_N\Psi_N^{(1)}$ we find that

$$\langle \Psi_N^{(1)}, H_N\Psi_N^{(1)}\rangle = Ne_{\rm H} + \langle U_N\Psi_N^{(1)}, \mathbb{H}_{\rm Bog}U_N\Psi_N^{(1)}\rangle + \mathcal{O}(N^{-1/2}).$$

By the variational principle,

$$\langle U_N\Psi_N^{(1)}, \mathbb{H}_{\rm Bog}U_N\Psi_N^{(1)}\rangle \geq \mu_1(\mathbb{H}_{\rm Bog})$$

we conclude the lower bound

$$\mu_1(H_N) \geq Ne_{\rm H} + \mu_1(\mathbb{H}_{\rm Bog}) + \mathcal{O}(N^{-1/2}).$$

Step 2: Ground state energy - upper bound. Let $\Phi^{(1)} \in \mathcal{F}(\mathscr{H}_+)$ be the ground state for $\mathbb{H}_{\rm Bog}$. We know that $\Phi^{(1)}$ is a quasi-free state, and in particular

$$\langle \Phi^{(1)}, \mathcal{N}_+^2\Phi^{(1)}\rangle \leq C < \infty.$$

We can restrict Φ to the truncated Fock space $\mathcal{F}^{\leq N}(\mathscr{H}_+)$ without changing the energy too much.

Exercise. *Let $\Phi \in \mathcal{F}(\mathscr{H}_+)$ be an eigenfunction for $\mathbb{H}_{\rm Bog}$. Define*

$$\Phi_N := \frac{\mathbb{1}^{\leq N}\Phi}{\|\mathbb{1}^{\leq N}\Phi\|} \in \mathcal{F}^{\leq N}(\mathscr{H}_+).$$

Prove that $\|\mathbb{1}^{\leq N}\Phi\| \to 1$ and

$$\lim_{N\to\infty}\langle \Phi_N, \mathbb{H}_{\rm Bog}\Phi_N\rangle = \langle \Phi, \mathbb{H}_{\rm Bog}\Phi\rangle.$$

By applying the above operator bound on $U_N(H_N - Ne_{\rm H})U_N^* - \mathbb{H}_{\rm Bog}$ for

$$\widetilde{\Phi}_N^{(1)} := \frac{\mathbb{1}^{\leq N}\Phi^{(1)}}{\|\mathbb{1}^{\leq N}\Phi^{(1)}\|} \in \mathcal{F}^{\leq N}(\mathscr{H}_+)$$

and using the variational principle for H_N we obtain the upper bound

$$\begin{aligned}\mu_1(H_N) \le \langle U_N^* \widetilde{\Phi}_N^{(1)}, H_N U_N^* \widetilde{\Phi}_N^{(1)} \rangle &= N e_{\rm H} + \langle \widetilde{\Phi}_N^{(1)}, \mathbb{H}_{\rm Bog} \widetilde{\Phi}_N^{(1)} \rangle + \mathcal{O}(N^{-1/2}) \\ &= N e_{\rm H} + \mu_1(\mathbb{H}_{\rm Bog}) + o(1)_{N\to\infty}.\end{aligned}$$

Combining with the lower bound in Step 1, we conclcude the convergence of the ground state energy

$$\mu_1(H_N) = N e_{\rm H} + \mu_1(\mathbb{H}_{\rm Bog}) + o(1)_{N\to\infty}.$$

Step 3: Convergence of ground state. Let $\Psi_N^{(1)}$ be a ground state of H_N. From Step 1 and Step 2 we know that

$$\mu_1(H_N) = \langle \Psi_N^{(1)}, H_N \Psi_N^{(1)} \rangle = N e_{\rm H} + \langle U_N \Psi_N^{(1)}, \mathbb{H}_{\rm Bog} U_N \Psi_N^{(1)} \rangle + o(1)$$

and

$$\mu_1(H_N) = N e_{\rm H} + \mu_1(\mathbb{H}_{\rm Bog}) + o(1)_{N\to\infty}.$$

Therefore,

$$\lim_{N\to\infty} \langle U_N \Psi_N^{(1)}, \mathbb{H}_{\rm Bog} U_N \Psi_N^{(1)} \rangle = \mu_1(\mathbb{H}_{\rm Bog}).$$

On the other hand, we know that $\mathbb{H}_{\rm Bog}$ has a unique ground state $\Phi^{(1)} \in \mathcal{F}(\mathscr{H}_+)$ (up to a phase) and there is the spectral gap

$$\mu_2(\mathbb{H}_{\rm Bog}) > \mu_1(\mathbb{H}_{\rm Bog}).$$

The convergence $U_N \Psi_N^{(1)} \to \Phi^{(1)}$ (up to a correct choice of the phase) thus follows from a standard variational technique.

Exercise. *Let A be a self-adjoint operator on a Hilbert space with the min-max values satisfying $\mu_1(A) < \mu_2(A)$. In particular, A has a unique ground state u_0 (up to a phase). Prove that for any sequence $\{x_n\}_{n\ge1} \subset Q(A)$ satisfying*

$$\|x_n\| = 1, \quad \langle x_n, A x_n \rangle \to \mu_1(A)$$

we can find a sequence of complex numbers $\{z_n\}$, $|z_n| = 1$ such that $z_n x_n \to u_0$ strongly.

Step 4: Higher eigenvalues - lower bound. Now we consider the lower bound for the eigenvalue $\mu_L(H_N)$. By the min-max principle, we have

$$\mu_L(H_N) = \max_{\Psi\in X, \|\Psi\|=1} \langle \Psi, H_N \Psi\rangle$$

where $X \subset D(H_N) \subset \mathscr{H}^{\otimes_s N}$ is a subspace spanned by the first L eigenfunctions $\Psi_N^{(1)}$, ... , $\Psi_N^{(L)}$ of H_N. Denote

$$\Phi_N^{(i)} := U_N \Psi_N^{(i)}, \quad Y = \mathrm{Span}\{\Phi_N^{(i)} : i = 1,2,...,L\} = U_N X \subset \mathcal{F}^{\leq N}(\mathscr{H}_+).$$

Then we have

$$\dim Y = \dim X = L$$

because U_N is a unitary operator from $\mathscr{H}^{\otimes_s N}$ to $\mathcal{F}^{+\leq N}(\mathscr{H}_+)$. Moreover, for any $i = 1, 2, ..., L$ we have

$$\langle \Phi_N^{(i)}, \mathcal{N}_+^2 \Phi_N^{(i)}\rangle = \langle \Psi_N^{(i)}, \mathcal{N}_+^2 \Psi_N^{(i)}\rangle = \mathcal{O}(1).$$

Therefore,

$$\max_{\Phi\in Y, \|\Phi\|=1} \langle \Phi, \mathcal{N}_+^2 \Phi\rangle = \mathcal{O}(1).$$

Using the operator bound

$$\pm \mathbb{1}^{\leq N}\Big(U_N (H_N - N e_{\mathrm{H}}) U_N^* - \mathbb{H}_{\mathrm{Bog}}\Big)\mathbb{1}^{\leq N} \leq C N^{-1/2}(\mathcal{N}_+^2 + 1).$$

we obtain

$$\max_{\Phi\in Y, \|\Psi\|=1} \Big| \langle \Phi, U_N H_N U_N^* \rangle - N e_{\mathrm{H}} - \langle \Phi, \mathbb{H}_{\mathrm{Bog}} \Phi\rangle \Big| \leq \mathcal{O}(N^{-1/2}).$$

Consequently, by the min-max principle we conclude that

$$\begin{aligned}
\mu_L(\mathbb{H}_{\mathrm{Bog}}) \leq \max_{\Phi\in Y, \|\Psi\|=1} \langle \Phi, \mathbb{H}_{\mathrm{Bog}}\Phi\rangle &\leq \max_{\Phi\in Y, \|\Psi\|=1} \langle \Phi, U_N H_N U_N^* \Phi\rangle - N e_{\mathrm{H}} + \mathcal{O}(N^{-1/2}) \\
&\leq \max_{\Psi\in X, \|\Psi\|=1} \langle \Psi, H_N \Psi\rangle - N e_{\mathrm{H}} + \mathcal{O}(N^{-1/2}) \\
&= \mu_L(H_N) - N e_{\mathrm{H}} + \mathcal{O}(N^{-1/2}).
\end{aligned}$$

Thus we obtain the desired lower bound

$$\mu_L(H_N) \geq N e_{\mathrm{H}} + \mu_L(\mathbb{H}_{\mathrm{Bog}}) + \mathcal{O}(N^{-1/2}).$$

Step 5: Higher eigenvalues - upper bound. We use the min-max principle again. Let

$\Phi^{(1)}$, ... , $\Phi^{(L)}$ be the first L eigenfunctions of $\mathbb{H}_{\rm Bog}$. Define

$$\widetilde{\Phi}_N^{(j)} := \frac{\mathbb{1}^{\leq N}\Phi^{(j)}}{\|\mathbb{1}^{\leq N}\Phi^{(j)}\|}, \quad j = 1, 2, ..., L.$$

Then by an extension of a previous exercise we know that for all $i, j \in \{1, 2, ..., L\}$,

$$\lim_{N\to\infty}\langle \widetilde{\Phi}_N^{(i)}, \widetilde{\Phi}_N^{(j)}\rangle = \langle \Phi^{(i)}, \Phi^{(j)}\rangle = \delta_{i=j}$$

and

$$\lim_{N\to\infty}\langle \widetilde{\Phi}_N^{(i)}, \mathbb{H}_{\rm Bog}\widetilde{\Phi}_N^{(j)}\rangle = \langle \Phi^{(i)}, \mathbb{H}_{\rm Bog}\Phi^{(j)}\rangle = \delta_{i=j}\mu_i(\mathbb{H}_{\rm Bog}).$$

Consequently, the space

$$\widetilde{Y} := \mathrm{Span}\{\widetilde{\Phi}_N^{(i)}, i = 1, 2, ..., L\} \subset \mathcal{F}^{\leq N}(\mathscr{H}_+)$$

satisfies

$$\dim \widetilde{Y} = L, \quad \lim_{N\to\infty}\max_{\Phi\in\widetilde{Y}, \|\Phi\|=1}\langle \Phi, \mathbb{H}_{\rm Bog}\Phi\rangle = \mu_L(\mathbb{H}_{\rm Bog}).$$

Since for any $i = 1, 2, ..., L$

$$\langle \widetilde{\Phi}_N^{(i)}, \mathcal{N}_+^2\widetilde{\Phi}_N^{(i)}\rangle \leq \langle \Psi^{(i)}, \mathcal{N}_+^2\Psi^{(i)}\rangle = \mathcal{O}(1), \quad \forall i = 1, 2, ..., L$$

we have

$$\max_{\Phi\in\widetilde{Y}, \|\Phi\|=1}\langle \Phi, \mathcal{N}_+^2\Phi\rangle = \mathcal{O}(1).$$

Thus from the operator bound

$$\pm\mathbb{1}^{\leq N}\Big(U_N(H_N - Ne_{\rm H})U_N^* - \mathbb{H}_{\rm Bog}\Big)\mathbb{1}^{\leq N} \leq CN^{-1/2}(\mathcal{N}_+^2 + 1).$$

we obtain

$$\max_{\Phi\in\widetilde{Y}, \|\Psi\|=1}\Big|\langle \Phi, U_N H_N U_N^*\rangle - Ne_{\rm H} - \langle \Phi, \mathbb{H}_{\rm Bog}\Phi\rangle\Big| \leq \mathcal{O}(N^{-1/2}).$$

By the min-max principle we conclude that

$$\begin{aligned}\mu_L(\mathbb{H}_{\rm Bog}) = \max_{\Phi\in\widetilde{Y}, \|\Psi\|=1}\langle \Phi, \mathbb{H}_{\rm Bog}\Phi\rangle &\geq \max_{\Phi\in\widetilde{Y}, \|\Psi\|=1}\langle \Phi, U_N H_N U_N^*\Phi\rangle - Ne_{\rm H} + \mathcal{O}(N^{-1/2}) \\ &\geq \mu_L(H_N) - Ne_{\rm H} + \mathcal{O}(N^{-1/2})\end{aligned}$$

which is equivalent to the upper bound

$$\mu_L(H_N) \leq N e_{\mathrm{H}} + \mu_L(\mathbb{H}_{\mathrm{Bog}})\mathcal{O}(N^{-1/2}).$$

Combining with the lower bound in Step 4, we obtain the convergence of eigenvalues

$$\mu_L(H_N) = N e_{\mathrm{H}} + \mu_L(\mathbb{H}_{\mathrm{Bog}}) + \mathcal{O}_L(N^{-1/2}).$$

Step 6: Convergence of eigenfunctions. In Step 4 we have proved that if $\Psi_N^{(1)}, \dots, \Psi_N^{(L)}$ are the first L eigenfunctions of H_N, then the vectors

$$\Phi_N^{(i)} := U_N \Psi_N^{(i)} \in \mathcal{F}^{\leq N}(\mathscr{H}_+)$$

satisfies

$$\langle \Phi_N^{(i)}, \Phi_N^{(j)} \rangle = \delta_{i=j}, \quad \lim_{N\to\infty} \langle \Phi_N^{(i)}, \mathbb{H}_{\mathrm{Bog}} \Phi_N^{(i)} \rangle = \mu_i(\mathbb{H}_{\mathrm{Bog}}), \quad \forall i,j \in \{1,2,...,L\}.$$

This implies that up to a subsequence as $N \to \infty$, the sequence $\{\Phi_N^{(L)}\}_N$ converges strongly to an eigenfunction of $\mathbb{H}_{\mathrm{Bog}}$ with eigenvalue $\mu_L(\mathbb{H}_{\mathrm{Bog}})$, thanks to the following abstract result (recall that $\mathbb{H}_{\mathrm{Bog}}$ has compact resolvent). This completes the proof of the theorem. *q.e.d.*

Exercise. *Let A be a self-adjoint operator on a Hilbert space. Assume that A is bounded from below and that the first L min-max values satisfy*

$$\mu_1 \leq \mu_2 \leq \dots \leq \mu_L < \inf \sigma_{\mathrm{ess}}(A).$$

Consider the vectors $\{x_n^j\}_{n\geq 1}^{1\leq j\leq L}$ satisfying

$$\lim_{n\to\infty} \langle x_n^i, x_n^j \rangle = \delta_{i=j}, \quad \lim_{n\to\infty} \langle x_n^j, A x_n^j \rangle = \mu_j, \quad \forall i,j \in \{1,2,...,L\}.$$

Prove that up to a subsequence as $n \to \infty$, the sequence $\{x_n^L\}_n$ converges strongly to an eigenfunction of A with eigenvalue μ_L.

7.7 Extension to singular interaction potentials

In this section, let us quickly explain how to adapt the previous strategy to justify Bogoliubov's approximation for singular interaction potentials. We consider the Hamiltonian

$$H_N = \sum_{i=1}^{N}(-\Delta_{x_i} + V(x_i)) + \frac{1}{N-1}\sum_{1\le i<j\le N} w(x_i - x_j)$$

acting on $\mathscr{H}^{\otimes_s N}$, $\mathscr{H} = L^2(\mathbb{R}^d)$.

Assumptions. In this section we make the following assumptions.

- $w, V_- \in L^p(\mathbb{R}^d) + L^\infty(\mathbb{R}^d)$, $V_+ \in L^p_{\rm loc}(\mathbb{R}^d)$ for some $p > \max(d/2, 2)$.
- The Hartree minimizer $u_0 \ge 0$ is unique (up to a phase) and **non-degenerate**:

  $$\begin{pmatrix} h + K_1 & K_2 \\ K_2^* & J(h+K_1)J^* \end{pmatrix} \ge \varepsilon_0 > 0 \quad \text{on} \quad \mathscr{H}_+ \oplus \mathscr{H}_+^*.$$

  Recall that $h = -\Delta + V + |u_0|^2 * w - \mu$, $K_1 := QKQ : \mathscr{H}_+ \to \mathscr{H}_+$, $K_2 = QKJQJ^* : \mathscr{H}_+^* \to \mathscr{H}_+$ with K the operator on $\mathscr{H}$ with kernel $K(x, y) = u_0(x)w(x-y)u_0(y)$.
- Any minimizing sequence of the Hartree functional has a subsequence converging to u_0 (up to a phase) strongly in $L^2(\mathbb{R}^d)$.

Remarks:

- The first condition on the potentials ensures that H_N is a self-adjoint operator in the same domain of the non-interacting Hamiltonian, by Kato-Rellich theorem. In particular, Coulomb potential $w(x) = 1/|x|$ with $x \in \mathbb{R}^3$ is allowed.
- The second condition means that the Hessian of the Hartree functional at the minimizer u_0 is non-degenerate. This ensures that the Bogoliubov Hamiltonian is well defined (see below).
- The third condition ensures that we have the complete BEC: for $\langle \Psi_N, H_N \Psi_N\rangle = Ne_{\rm H} + o(N)$,

  $$\lim_{N\to\infty} \frac{\langle u_0, \gamma^{(1)}_{\Psi_N} u_0\rangle}{N} = 1.$$

Recall the Bogoliubov Hamiltonian

$$\mathbb{H}_{\rm Bog} = \sum_{m,n\ge 1} \langle u_m, (h+K)u_n\rangle a_m^* a_n + \frac{1}{2}\sum_{m,n\ge 1}\Big(\langle u_m, KJu_n\rangle a_m^* a_n^* + h.c.\Big)$$

on the excited Fock space $\mathcal{F}(\mathscr{H}_+)$, where $a_n = a(u_n)$ with $\{u_n\}_{n=0}^\infty$ an orthonormal basis for $\mathscr{H} = L^2(\mathbb{R}^d)$.

Theorem. *Under the above assumptions, the Bogoliubov Hamiltonian $\mathbb{H}_{\rm Bog}$ on the excited Fock space $\mathcal{F}(\mathscr{H}_+)$ is a self-adjoint operator with the same quadratic form domain of $\mathrm{d}\Gamma(h)_{|\mathcal{F}(\mathscr{H}_+)}$. Moreover,*

- *There exist a Bogoliubov transformation $\mathbb{U}$ on $\mathcal{F}(\mathscr{H}_+)$ and a self-adjoint operator $\xi > 0$ on $\mathscr{H}_+$ such that*

$$\mathbb{U}^*\mathbb{H}_{\rm Bog}\mathbb{U} = \mathrm{d}\Gamma(\xi) + \mu_1(\mathbb{H}_{\rm Bog}).$$

  Moreover, $\inf\sigma(\xi) > 0$ *and* $\sigma_{\rm ess}(\xi) = \sigma_{\rm ess}(h_{|\mathscr{H}_+})$.

- *$\mathbb{H}_{\rm Bog}$ has a unique ground state $\mathbb{U}\Omega$ (up to a complex phase). Moreover, it has the spectral gap between the second and the first min-max values*

$$\mu_2(\mathbb{H}_{\rm Bog}) - \mu_1(\mathbb{H}_{\rm Bog}) = \inf\sigma(\xi) > 0.$$

- *We have the operator lower bound*

$$\mathbb{H}_{\rm Bog} \ge \frac{1}{C}\mathrm{d}\Gamma(Q(-\Delta + V_+ + 1)Q) - C.$$

Proof. **Step 1.** From the condition $w \in L^p(\mathbb{R}^d) + L^\infty(\mathbb{R}^d)$ and $u_0 \in H^1(\mathbb{R}^d)$ we find that K is a Hilbert-Schmidt operator

$$\|K\|_{\rm HS}^2 = \iint_{\mathbb{R}^d\times\mathbb{R}^d} |K(x,y)|^2 \mathrm{d}x\mathrm{d}y = \iint_{\mathbb{R}^d\times\mathbb{R}^d} |u_0(x)|^2|w(x-y)|^2|u_0(y)|^2\mathrm{d}x\mathrm{d}y < \infty.$$

To see the the latter bound we can use Sobolev embedding $H^1(\mathbb{R}^d) \subset L^q(\mathbb{R}^d)$ for $2 \le q < 2^*$ (recall $2^* = +\infty$ if $d \le 2$ and $2^* = 2d/(d-2)$ if $d \ge 3$) and Young's inequality. More precisely, by linearity we can assume $w \in L^r(\mathbb{R}^d)$ with $\max(d/2,2) < r \leq \infty$ and estimate

$$\iint_{\mathbb{R}^d\times\mathbb{R}^d} |u_0(x)|^2|w(x-y)|^2|u_0(y)|^2 \mathrm{d}x\mathrm{d}y \leq \|u_0\|^2_{L^q(\mathbb{R}^d)}\|w\|^2_{L^r(\mathbb{R}^d)}\|u_0\|^2_{L^q(\mathbb{R}^d)}$$

with

$$q,r \geq 2, \quad \frac{1}{q}+\frac{1}{r}+\frac{1}{q} = 1.$$

The condition $r > \max(d/2,2)$ allows us to take $q < 2^*$.

Step 2. Since K is Hilbert-Schmidt, K_1 and K_2 are also Hilbert-Schmidt operators. Thanks to the non-degeneracy of the Hessian

$$\mathcal{A} := \begin{pmatrix} h+K_1 & K_2 \\ K_2^* & J(h+K_1)J^* \end{pmatrix} \geq \varepsilon_0 > 0 \quad \text{on} \quad \mathscr{H}_+ \oplus \mathscr{H}_+^*,$$

we can apply the diagonalization procedure discussed in the previous chapter to

$$\mathbb{H}_{\rm Bog} = \sum_{m,n\geq 1} \langle u_m, (h+K_1)u_n\rangle a_m^* a_n + \frac{1}{2}\sum_{m,n\geq 1}\Big(\langle u_m, K_2 J u_n\rangle a_m^* a_n^* + h.c.\Big)$$

Thus there exist a Bogoliubov transformation $\mathbb{U}$ on $\mathcal{F}(\mathscr{H}_+)$ and a self-adjoint operator $\xi > 0$ on $\mathscr{H}_+$ such that

$$\mathbb{U}^*\mathbb{H}_{\rm Bog}\mathbb{U} = \mathrm{d}\Gamma(\xi) + \mu_1(\mathbb{H}_{\rm Bog})$$

Here the ground state energy $\mu_1(\mathbb{H}_{\rm Bog})$ is finite. Let us prove that

$$\sigma_{\rm ess}(\xi) = \sigma_{\rm ess}(\widetilde{h}), \quad \widetilde{h} := h + K_1.$$

In fact, from the diagonalization procedure we also know that there exists a block operator

$$\mathcal{V} = \begin{pmatrix} U & V \\ JVJ & JUJ^* \end{pmatrix} \in \mathscr{G}$$

(which is associated to $\mathbb{U}$) such that

$$\begin{pmatrix} \xi & 0 \\ 0 & J\xi J^* \end{pmatrix} = \mathcal{V}\mathcal{A}\mathcal{V}^* = \begin{pmatrix} U & V \\ JVJ & JUJ^* \end{pmatrix}\begin{pmatrix} \widetilde{h} & K_2 \\ K_2^* & J\widetilde{h}J^* \end{pmatrix}\begin{pmatrix} U^* & J^*V^*J^* \\ V^* & JU^*J^* \end{pmatrix}$$

A direct computation shows that

$$\xi = U\widetilde{h}U^* + UK_2V^* + VK_2^*U^* + VJ\widetilde{h}J^*V^*.$$

Since U is bounded and V, K_2 are Hilbert-Schmidt, UK_2V^* and $VK_2^*U^*$ are trace class. Moreover, by a lemma from the proof of the diagonalization of quadratic Hamiltonians, we know that

$$\mathrm{Tr}(X^{1/2}\widetilde{h}X^{1/2}) < \infty, \quad X := J^*V^*VJ.$$

The latter implies that

$$\|\widetilde{h}^{1/2}J^*V^*\|_{\mathrm{HS}}^2 = \mathrm{Tr}(\widetilde{h}^{1/2}J^*V^*VJ\widetilde{h}^{1/2}) = \mathrm{Tr}(\widetilde{h}^{1/2}X\widetilde{h}^{1/2}) < \infty$$

and similarly $\|VJ\widetilde{h}^{1/2}\|_{\mathrm{HS}} < \infty$. Thus $VJ\widetilde{h}J^*V^*$ is trace class. In summary, we have proved that $\xi - U\widetilde{h}U^*$ is a trace class operator, therefore

$$\sigma_{\mathrm{ess}}(\xi) = \sigma_{\mathrm{ess}}(U\widetilde{h}U^*).$$

Since $UU^* - 1$ and $U^*U - 1$ are trace class (thanks to Shale's condition), we deduce that

$$\sigma_{\mathrm{ess}}(\xi) = \sigma_{\mathrm{ess}}(U\widetilde{h}U^*) = \sigma_{\mathrm{ess}}(\widetilde{h}).$$

Exercise. *Let B be a self-adjoint operator on a Hilbert space. Let U be a bounded operator such that U^{-1} is bounded and $UU^* - 1$ is a compact operator. Prove that*

$$\sigma_{\mathrm{ess}}(UBU^*) = \sigma_{\mathrm{ess}}(B).$$

Hint: You can write $UBU^* - \lambda = U(B-\lambda)U^* + \lambda(UU^* - 1)$ for all $\lambda \in \mathbb{R}$.

Step 3. We have proved that

$$\sigma_{\mathrm{ess}}(\xi) = \sigma_{\mathrm{ess}}(\widetilde{h}) = \sigma_{\mathrm{ess}}(h + K_1).$$

Since K_1 is a Hilbert-Schmidt operator, we also obtain

$$\sigma_{\mathrm{ess}}(\xi) = \sigma_{\mathrm{ess}}(h + K_1) = \sigma_{\mathrm{ess}}(h).$$

Moreover, from the non-degeneracy condition on the Hessian $\mathcal{A} \geq \varepsilon_0$, we have

$$h + K_1 \geq \varepsilon_0 > 0.$$

Consequently,

$$\inf \sigma_{\text{ess}}(\xi) = \inf \sigma_{\text{ess}}(h + K_1) \geq \varepsilon_0 > 0.$$

Since $\xi > 0$, we deduce that

$$\inf \sigma(\xi) > 0.$$

In fact, if $\inf \sigma(\xi) = \inf \sigma_{\text{ess}}(\xi)$, then obviously $\inf \sigma(\xi) \geq \varepsilon_0 > 0$. On the other hand, if $\inf \sigma(\xi) < \inf \sigma_{\text{ess}}(\xi)$, then by the min-max principle, $\inf \sigma(\xi)$ is an eigenvalue of ξ, which must be strictly positive since $\xi > 0$ as an operator.

Step 4. Using

$$\mathbb{U}^* \mathbb{H}_{\text{Bog}} \mathbb{U} = \text{d}\Gamma(\xi) + \mu_1(\mathbb{H}_{\text{Bog}})$$

and $\inf \sigma(\xi) > 0$, we find that $\mathbb{H}_{\text{Bog}}$ has a unique ground state $\mathbb{U}\Omega$ (up to a phase). Moreover, it satisfies the spectral gap

$$\mu_2(\mathbb{H}_{\text{Bog}}) - \mu_1(\mathbb{H}_{\text{Bog}}) = \mu_2(\text{d}\Gamma(\xi)) - \mu_1(\text{d}\Gamma(\xi)) = \inf \sigma(\xi) > 0.$$

Step 5. Now we prove the operator lower bound for $\mathbb{H}_{\text{Bog}} - \mu_1(\mathbb{H}_{\text{Bog}})$. Since $\inf \sigma(\xi) > 0$, we have

$$\mathbb{U}^* \mathbb{H}_{\text{Bog}} \mathbb{U} - \mu_1(\mathbb{H}_{\text{Bog}}) = \text{d}\Gamma(\xi) \geq \inf \sigma(\xi) \mathcal{N}_+ \geq \frac{1}{C} \mathbb{U}^* (\mathcal{N}_+) \mathbb{U} - C.$$

In the second inequality, we have used

$$\mathbb{U}^* \mathcal{N}_+ \mathbb{U} \leq C(\mathcal{N}_+ + 1).$$

Thus we have proved that

$$\mathbb{H}_{\text{Bog}} \geq \frac{1}{C} \mathcal{N}_+ - C.$$

Next, let us consider the Bogoliubov Hamiltonian in more detail.

$$\mathbb{H}_{\text{Bog}} = \sum_{m,n \geq 1} \langle u_m, (h + K) u_n \rangle a_m^* a_n + \frac{1}{2} \sum_{m,n \geq 1} \Big(\langle u_m, K J u_n \rangle a_m^* a_n^* + h.c. \Big)$$

Since K is a Hilbert-Schmidt operator, we have

$$\pm\frac{1}{2}\sum_{m,n\geq 1}\Big(\langle u_m, KJu_n\rangle a_m^* a_n^* + h.c.\Big) \leq C(\mathcal{N}_+ + 1).$$

Moreover, the condition $V_-, w \in L^p(\mathbb{R}^d) + L^\infty(\mathbb{R}^d)$ with $p > \max(d/2, 2)$ ensures that

$$|V_-| + |u_0|^2 * |w| \leq \frac{1}{2}(-\Delta) + C.$$

Thus

$$h + K = -\Delta + V + |u_0|^2 * w - \mu + K \geq \frac{1}{2}(-\Delta + V_+ + 1) - C.$$

In the second quantization, we find that

$$\mathrm{d}\Gamma(h+K) \geq \frac{1}{2}\mathrm{d}\Gamma(-\Delta + V_+ + 1) - C\mathcal{N}_+.$$

Thus we conclude that

$$\mathbb{H}_{\rm Bog} \geq \frac{1}{2}\mathrm{d}\Gamma(-\Delta + V_+ + 1) - C(\mathcal{N}_+ + 1) \geq \frac{1}{2}\mathrm{d}\Gamma(-\Delta + V_+ + 1) - C(\mathbb{H}_{\rm Bog} + C)$$

which is equivalent to

$$\mathbb{H}_{\rm Bog} \geq \frac{1}{C}\mathrm{d}\Gamma(-\Delta + V_+ + 1) - C.$$

This completes the analysis of the Bogoliubov Hamiltonian. *q.e.d.*

Theorem. *Under the assumptions in the beginning of this section, the following statements hold true.*

- **Convergence of min-max values.** *For any $i = 1, 2, ...$, the i-th min-max value of H_N satisfies*

$$\lim_{N\to\infty}\Big(\mu_i(H_N) - Ne_{\rm H} - \mu_i(\mathbb{H}_{\rm Bog})\Big) = 0.$$

- **Convergence of eigenstates.** *Assume that $\mu_L(\mathbb{H}_{\rm Bog}) < \inf\sigma_{\rm ess}(\mathbb{H}_{\rm Bog})$ for some $L \geq 1$. Then $\mu_L(\mathbb{H}_{\rm Bog})$ is an eigenvalue for $\mathbb{H}_{\rm Bog}$ and for N large, $\mu_L(H_N)$ is an eigenvalue of H_N. Moreover, if $\Psi_N^{(L)}$ is an eigenfunction of H_N with eigenvalue*

$\mu_L(H_N)$, then up to a subsequence as $N \to \infty$, we have

$$\lim_{N\to\infty} U_N \Psi_N^{(L)} = \Phi^{(L)}$$

strongly in $\mathcal{F}(\mathscr{H}_+)$, where $\Phi^{(L)}$ is an eigenfunction of $\mathbb{H}_{\rm Bog}$ with eigenvalue $\mu_L(\mathbb{H}_{\rm Bog})$.

The proof of this theorem follows the general strategy we discuss before, namely we will compare $U_N(H_N - Ne_{\rm H})U_N^*$ with $\mathbb{H}_{\rm Bog}$. However, since the interaction potential w may be unbounded, the analysis is more complicated in several places. Here is a quick explanation of necessary modifications:

- We need to modify the operator bound on truncated Fock space. For example, we cannot use $|w| \le \|w\|_{L^\infty}$ anymore, and hence we cannot simply bound

  $$A := U_N(H_N - Ne_{\rm H})U_N^* - \mathbb{H}_{\rm Bog}$$

  in terms of $\mathcal{N}_+$. We have to use some kinetic part to control the error, resulting the following bound on $\mathcal{F}^{\le M}(\mathscr{H}_+)$ with $1 \ll M \le N$

  $$\pm \mathbb{1}^{\le M} A \mathbb{1}^{\le M} \le C\sqrt{\frac{M}{N}}(\mathbb{H}_{\rm Bog} + C).$$

- In order to put the previous bound to good use, we need a new tool to **localize the particle number on Fock space**. More precisely, we will write

  $$A \approx f_M A f_M + g_M A g_M,$$

  where $f_M \approx \mathbb{1}(\mathcal{N}_+ \le M)$ and $g_M \approx \mathbb{1}(\mathcal{N}_+ > M)$. This is an analogue of the IMS localization formula, but now the local functions $\varphi_j(x)$ with $x \in \mathbb{R}^d$ are replaced by functions of number operator $\mathcal{N}_+$. The part $f_M A f_M$ can be controlled by the above operator bound, provided that $M \ll N$. The part $g_M A g_M$ is bounded by the variational principle

  $$g_M A g_M \ge \mu_1(A) g_M^2 \ge \mu_1(A)\frac{\mathcal{N}_+}{M}.$$

  Thanks to the condensation $\langle \Phi, \mathcal{N}_+ \Phi\rangle \ll N$, if we choose

  $$\langle \Phi, \mathcal{N}_+ \Phi\rangle \ll M \ll N,$$

  then the contribution from $g_M A g_M$ can be controlled.

Now let us come to the details.

Lemma (Operator bound on truncated Fock space)**.** *Take* $1 \le M \le N$ *and denote* $\mathbb{1}^{\le M} := \mathbb{1}(\mathcal{N}_+ \le M)$*. Then we have the operator bound on* $\mathcal{F}^{\le M}(\mathscr{H}_+)$*:*

$$\pm \mathbb{1}^{\le M}\Big(U_N(H_N - Ne_{\rm H})U_N^* - \mathbb{H}_{\rm Bog}\Big)\mathbb{1}^{\le M} \le C\sqrt{\frac{M}{N}}\mathbb{1}^{\le M}(\mathbb{H}_{\rm Bog}+C)\mathbb{1}^{\le M}.$$

Proof. Recall that

$$U_N(H_N - Ne_{\rm H})U_N^* = \sum_{j=0}^{4} A_j$$

where

$$\begin{aligned}
A_0 &= \frac{1}{2}W_{0000}\frac{\mathcal{N}_+(\mathcal{N}_+-1)}{N-1},\\
A_1 &= \sum_{n\ge 1}\left(T_{0n} + W_{000n}\frac{N-\mathcal{N}_+-1}{N-1}\right)\sqrt{N-\mathcal{N}_+}a_n + h.c.,\\
A_2 &= \sum_{m,n\ge 1}\langle u_m, (h+K)u_n\rangle a_m^* a_n + \sum_{m,n\ge 1}\left\langle u_m, \left(|u_0|^2 * w + K\right)u_n\right\rangle a_m^* a_n \frac{1-\mathcal{N}_+}{N-1}\\
&\quad + \frac{1}{2}\sum_{m,n\ge 1}\left(\langle u_m, KJu_n\rangle a_n^* a_m^* \frac{\sqrt{(N-\mathcal{N}_+)(N-\mathcal{N}_+-1)}}{N-1} + h.c.\right),\\
A_3 &= \frac{1}{N-1}\sum_{m,n,p\ge 1} W_{mnp0}a_m^* a_n^* a_p \sqrt{N-\mathcal{N}_+} + h.c.,\\
A_4 &= \frac{1}{2(N-1)}\sum_{m,n,p,q\ge 1} W_{mnpq}a_m^* a_n^* a_p a_q.
\end{aligned}$$

We will estimate term by term.

Estimate A_0. We have

$$0 \le A_0 \le C\frac{\mathcal{N}_+^2}{N}.$$

When restricting to the subspace $\mathcal{F}^{\le M}(\mathscr{H}_+)$, we can use $\mathcal{N}_+ \le M$ to get

$$0 \le \mathbb{1}^{\le M}A_0\mathbb{1}^{\le M} \le C\frac{M}{N}\mathbb{1}^{\le M}\mathcal{N}_+\mathbb{1}^{\le M} \le C\sqrt{\frac{M}{N}}\mathbb{1}^{\le M}(\mathbb{H}_{\rm Bog}+C)\mathbb{1}^{\le M}.$$

Estimate A_1. We have proved that

$$\pm A_1 \le C\varepsilon^{-1}\frac{\mathcal{N}_+^2}{N} + \varepsilon\mathcal{N}_+, \quad \forall \varepsilon > 0.$$

Restricting to the subspace $\mathcal{F}^{\leq M}(\mathscr{H}_+)$ and taking $\varepsilon = \sqrt{M/N}$ and , we have

$$\pm\, \mathbb{1}^{\leq M} A_1 \mathbb{1}^{\leq M} \leq C \mathbb{1}^{\leq M}\Big(\varepsilon^{-1}\frac{M}{N}\mathcal{N}_+ + \varepsilon \mathcal{N}_+\Big) \leq C\sqrt{\frac{M}{N}}\mathbb{1}^{\leq M}(\mathbb{H}_{\rm Bog}+C)\mathbb{1}^{\leq M}.$$

Estimate A_2. We have proved that

$$\pm(A_2 - \mathbb{H}_{\rm Bog}) \leq C\frac{(\mathcal{N}_+ + 1)^2}{N}$$

as a quadratic form estimate on $\mathcal{F}^{\leq N}(\mathscr{H}_+)$. When restricting to the subspace $\mathcal{F}^{\leq M}(\mathscr{H}_+)$, we have

$$\pm \mathbb{1}^{\leq M}(A_2 - \mathbb{H}_{\rm Bog})\mathbb{1}^{\leq M} \leq C\frac{M}{N}\mathbb{1}^{\leq M}(\mathcal{N}_+ + 1) \leq C\sqrt{\frac{M}{N}}\mathbb{1}^{\leq M}(\mathbb{H}_{\rm Bog}+C)\mathbb{1}^{\leq M}.$$

Estimate A_4. We can interpret

$$\begin{aligned} A_4 &= \frac{1}{2(N-1)}\sum_{m,n,p,q\geq 1} W_{mnpq} a_m^* a_n^* a_p a_q \\ &= \frac{1}{2(N-1)}\sum_{m,n,p,q\geq 0} \langle u_m \otimes u_n, (Q\otimes QwQ\otimes Q) u_p \otimes u_q\rangle a_m^* a_n^* a_p a_q \end{aligned}$$

as the second quantization of the two-body operator $(N-1)^{-1} Q\otimes QwQ\otimes Q$ (here $w = w(x-y)$ is the multiplication operator). From the assumption $w \in L^p(\mathbb{R}^d) + L^\infty(\mathbb{R}^d)$ with $p > \max(d/2, 2)$ and Sobolev's embedding theorem we obtain the two-body inequality

$$|w(x-y)| \leq C(-\Delta_x - \Delta_y + 1).$$

Therefore,

$$\pm Q\otimes QwQ\otimes Q \leq C((Q(-\Delta+1)Q)\otimes Q + Q\otimes(Q(-\Delta+1)Q)).$$

Taking the second quantization we obtain

$$\pm A_4 \leq \frac{C}{N}\mathrm{d}\Gamma(Q(-\Delta+1)Q)\mathcal{N}_+$$

Projecting on the subspace $\mathcal{F}^{\leq M}(\mathscr{H}_+)$, we get

$$\pm \mathbb{1}^{\leq M} A_4 \mathbb{1}^{\leq M} \leq C\frac{M}{N}\mathbb{1}^{\leq M}\mathrm{d}\Gamma(Q(-\Delta+1)Q) \leq C\sqrt{\frac{M}{N}}\mathbb{1}^{\leq M}(\mathbb{H}_{\rm Bog}+C)\mathbb{1}^{\leq M}.$$

Estimate A_3**.** Finally, we consider

$$
\begin{aligned}
A_3 &= \frac{1}{N-1} \sum_{m,n,p \geq 1} W_{mnp0} a_m^* a_n^* a_p \sqrt{N - \mathcal{N}_+} + h.c. \\
&= \frac{1}{N-1} U_N \Big(\sum_{m,n,p,q \geq 0} \langle u_m \otimes u_n, (Q \otimes QwQ \otimes P) u_p \otimes u_q \rangle a_m^* a_n^* a_p a_q + h.c. \Big) U_N^*
\end{aligned}
$$

Thus up to a transformation by U_N, A_3 is the second quantization of the two-body operator

$$
(N-1)^{-1} \Big(Q \otimes QwQ \otimes P + Q \otimes QwP \otimes Q + h.c. \Big).
$$

From the assumption $w \in L^p(\mathbb{R}^d) + L^\infty(\mathbb{R}^d)$ with $p > \max(d/2, 2)$ and Sobolev's embedding theorem we obtain the two-body inequality

$$
\begin{aligned}
&\pm \Big(Q \otimes QwQ \otimes P + Q \otimes QwP \otimes Q + h.c. \Big) \\
&\leq 2\varepsilon^{-1} Q \otimes Q|w|Q \otimes Q + \varepsilon \Big(Q \otimes P|w|Q \otimes P + P \otimes Q|w|P \otimes Q \Big), \\
&\leq C\varepsilon^{-1} \Big((Q(-\Delta+1)Q) \otimes Q + Q \otimes (Q(-\Delta+1)Q) \Big) \\
&\quad + C\varepsilon \Big((Q(-\Delta+1)Q) \otimes P + P \otimes (Q(-\Delta+1)Q) \Big), \quad \forall \varepsilon > 0.
\end{aligned}
$$

In the second quantization form, we obtain

$$
\pm A_3 \leq \frac{C}{N} \Big(\varepsilon^{-1} \mathcal{N}_+ + \varepsilon N \Big) \mathrm{d}\Gamma(Q(-\Delta+1)Q).
$$

Restricting to $\mathcal{F}^{\leq M}(\mathscr{H}_+)$ and choosing $\varepsilon = \sqrt{M/N}$ we get

$$
\pm \mathbb{1}^{\leq M} A_3 \mathbb{1}^{\leq M} \leq \frac{C}{N} \Big(\varepsilon^{-1} M + \varepsilon N \Big) \mathbb{1}^{\leq M} \mathrm{d}\Gamma(Q(-\Delta+1)Q) \leq C \sqrt{\frac{M}{N}} \mathbb{1}^{\leq M} (\mathbb{H}_{\mathrm{Bog}} + C) \mathbb{1}^{\leq M}.
$$

Thus in summary, we have prove that

$$
\pm \mathbb{1}^{\leq M} \Big(U_N (H_N - N e_{\mathrm{H}}) U_N^* - \mathbb{H}_{\mathrm{Bog}} \Big) \mathbb{1}^{\leq M} \leq C \sqrt{\frac{M}{N}} \mathbb{1}^{\leq M} (\mathbb{H}_{\mathrm{Bog}} + C) \mathbb{1}^{\leq M}.
$$

This completes the proof of the lemma. *q.e.d.*

Lemma (IMS formula on Fock space)**.** *Let A be a non–negative operator on a bosonic Fock space $\mathcal{F}(\mathscr{H})$ such that $P_i D(A) \subset D(A)$ and $P_i A P_j = 0$ if $|i-j| > \ell$, where*

$P_i = \mathbb{1}(\mathcal{N} = i)$. Let $f, g : \mathbb{R} \to [0,1]$ be smooth functions such that $f^2 + g^2 = 1$, $f(x) = 1$ for $x \le 1/2$ and $f(x) = 0$ for $x \ge 1$. For any $M \ge 1$ define

$$f_M := f(\mathcal{N}/M)\,, \qquad g_M := g(\mathcal{N}/M)\,.$$

Then

$$\pm\Big(A - f_M A f_M - g_M A g_M\Big) \le (\|f'\|^2_{L^\infty} + \|g'\|^2_{L^\infty})\frac{\ell^3}{M^2}[A]_{\text{diag}}$$

with the "diagonal part"

$$[A]_{\text{diag}} := \sum_{i=0}^{\infty} P_i A P_i.$$

Proof. We start from the "IMS-identity"

$$A - f_M A f_M - g_M A g_M = \frac{1}{2}\left([[A, f_M], f_M]] + [[A, g_M], g_M]]\right)$$

which follows from the "double commutator identities"

$$[[A, f_M], f_M] = f_M^2 A + A f_M^2 - 2 f_M A f_M,$$
$$[[A, g_M], g_M] = g_M^2 A + A g_M^2 - 2 g_M A g_M.$$

By decomposing further

$$\mathbb{1}_{\mathcal{F}(\mathscr{H})} = \sum_{i=0}^{\infty} P_i$$

we find that

$$\begin{aligned}
[[A, f_M], f_M]] &= \sum_{i,j=0}^{\infty} P_i[[A, f_M], f_M]] P_j = \sum_{i,j=0}^{\infty} \Big(f_M^2(i) + f_M^2(j) - 2 f_M(i) f_M(j)\Big) P_i A P_j \\
&= \sum_{i,j=0}^{\infty} \Big(f_M(i) - f_M(j)\Big)^2 P_i A P_j = \sum_{1 \le |i-j| \le \ell}^{\infty} \Big(f(i/M) - f(j/M)\Big)^2 P_i A P_j.
\end{aligned}$$

In the last equality we have used the assumption that $P_i A P_j = 0$ if $|i - j| > \ell$. Combining with a similar formula for g_M, we arrive at

$$A - f_M A f_M - g_M A g_M = \frac{1}{2} \sum_{1 \le |i-j| \le \ell}^{\infty} \Big[(f(i/M) - f(j/M))^2 + (g(i/M) - g(j/M))^2\Big] P_i A P_j.$$

Since f, g are smooth, we have the uniform bound for all $|i-j| \le \ell$:

$$(f(i/M) - f(j/M))^2 + (g(i/M) - g(j/M))^2 \le (\|f'\|_{L^\infty}^2 + \|g'\|_{L^\infty}^2)\frac{\ell^2}{M^2}.$$

On the other hand, since $A \ge 0$ we have the Cauchy-Schwarz inequality

$$\pm(P_i A P_j + h.c.) \le P_i A P_i + P_j A P_j.$$

Thus we conclude that

$$\begin{aligned}
&\pm\Big(A - f_M A f_M - g_M A g_M\Big)\\
&= \pm\frac{1}{4}\sum_{1\le|i-j|\le\ell}^{\infty}\Big[(f(i/M) - f(j/M))^2 + (g(i/M) - g(j/M))^2\Big](P_i A P_j + P_j A P_i)\\
&\le \frac{1}{4}(\|f'\|_{L^\infty}^2 + \|g'\|_{L^\infty}^2)\frac{\ell^2}{M^2}\sum_{1\le|i-j|\le\ell}^{\infty}(P_i A P_i + P_j A P_j)\\
&\le (\|f'\|_{L^\infty}^2 + \|g'\|_{L^\infty}^2)\frac{\ell^3}{M^2}\sum_{i=0}^{\infty} P_i A P_i.
\end{aligned}$$

This completes the proof of the lemma. *q.e.d.*

Exercise. *Prove that*

$$[\mathbb{H}_{\rm Bog}]_{\rm diag} \le C(\mathbb{H}_{\rm Bog} + C)$$

and

$$[U_N H_N U_N^*]_{\rm diag} \le C(U_N H_N U_N^* + CN).$$

Hint: For the second bound you can use $H_N \ge (1-\varepsilon)\sum_{i=1}^N(-\Delta + V)_i - C_\varepsilon N$.

Now we are ready to provide

Proof of the theorem. **Step 1. Ground state energy - lower bound.** Denote

$$\widetilde{H}_N = U_N(H_N - N e_{\rm H})U_N^*.$$

Let us prove that

$$\mu_1(\widetilde{H}_N) \ge \mu_1(\mathbb{H}_{\rm Bog}) + o(1)_{N\to\infty}.$$

By applying the localization formula for $A = \widetilde{H}_N - \mu_1(\widetilde{H}_N)$, with $\ell = 2$ and $1 \ll M \ll N$ we have the operator inequality

$$\widetilde{H}_N \geq f_M \widetilde{H}_N f_M + g_M \widetilde{H}_N g_M - \frac{C}{M^2}[\widetilde{H}_N - \mu_1(\widetilde{H}_N)]_{\text{diag}}.$$

The main part $f_M \widetilde{H}_N f_M$ satisfies the operator bound on truncated Fock space

$$\pm f_M \Big(\widetilde{H}_N - \mathbb{H}_{\text{Bog}}\Big) f_M \leq C\sqrt{\frac{M}{N}} f_M(\mathbb{H}_{\text{Bog}} + C) f_M$$

which implies that

$$f_M \widetilde{H}_N f_M \geq \Big(1 - C\sqrt{\frac{M}{N}}\Big) f_M \mathbb{H}_{\text{Bog}} f_M - C\sqrt{\frac{M}{N}} f_M^2.$$

Using the variational principle $\mathbb{H}_{\text{Bog}} \geq \mu_1(\mathbb{H}_{\text{Bog}}) > -\infty$ we find that

$$\begin{aligned} f_M \widetilde{H}_N f_M &\geq \Big(1 - C\sqrt{\frac{M}{N}}\Big) \mu_1(\mathbb{H}_{\text{Bog}}) f_M^2 - C\sqrt{\frac{M}{N}} f_M^2 \\ &\geq \Big[\mu_1(\mathbb{H}_{\text{Bog}}) - C\sqrt{\frac{M}{N}}\Big] f_M^2. \end{aligned}$$

The part $g_M \widetilde{H}_N g_M$ can be bounded from below by the variational principle

$$g_M \widetilde{H}_N g_M \geq \mu_1(\widetilde{H}_N) g_M^2 = \mu_1(\widetilde{H}_N)(1 - f_M^2).$$

The localization error is controlled by the rough estimate

$$[U_N H_N U_N^*]_{\text{diag}} \leq C(U_N H_N U_N^* + CN)$$

which implies

$$[\widetilde{H}_N]_{\text{diag}} \leq C(\widetilde{H}_N + CN), \quad |\mu_1(\widetilde{H}_N)| \leq CN.$$

In summary, we have the operator inequality on $\mathcal{F}^{\leq N}(\mathscr{H}_+)$

$$\begin{aligned} \widetilde{H}_N &\geq f_M \widetilde{H}_N f_M + g_M \widetilde{H}_N g_M - \frac{C}{M^2}[\widetilde{H}_N - \mu_1(\widetilde{H}_N)]_{\text{diag}} \\ &\geq \Big[\mu_1(\mathbb{H}_{\text{Bog}}) - C\sqrt{\frac{M}{N}}\Big] f_M^2 + \mu_1(\widetilde{H}_N)(1 - f_M^2) - \frac{C}{M^2}(\widetilde{H}_N) + CN) \end{aligned}$$

which is equivalent to

$$(1+CM^{-2})\widetilde{H}_N \geq \left[\mu_1(\mathbb{H}_{\rm Bog}) - C\sqrt{\frac{M}{N}}\right] f_M^2 + \mu_1(\widetilde{H}_N)(1-f_M^2) - \frac{CN}{M^2}.$$

By the assumption on the condensation, we can take a wave function $\Psi_N \in \mathscr{H}^{P\otimes N}$ such that

$$\langle \Psi_N, H_N \Psi_N\rangle \leq \mu_1(H_N) + N^{-1}, \quad \varepsilon_N := \frac{\langle \Psi_N, \mathcal{N}_+ \Psi_N\rangle}{N} = o(1)_{N\to\infty}.$$

Equivalently, the vector $U_N\Psi_N \in \mathcal{F}^{\leq N}(\mathscr{H}_+)$ satisfies

$$\langle \Phi_N, \widetilde{H}_N \Phi_N\rangle \leq \mu_1(\widetilde{H}_N) + N^{-1}, \quad \langle \Phi_N, \mathcal{N}_+ \Phi_N\rangle = \varepsilon_N N = o(N)_{N\to\infty}.$$

In particular, if we choose

$$\max\{\varepsilon_N N, N^{1/2}\} \ll M \ll N$$

then

$$0 \leq \langle \Phi_N, g_M^2 \Phi_N\rangle \leq \langle \Phi_N, (\mathcal{N}_+/M)\Phi_N\rangle = o(1)_{N\to\infty}$$

and hence

$$\langle \Phi_N, f_M^2 \Phi_N\rangle = 1 - \langle \Phi_N, g_M^2 \Phi_N\rangle = 1 + o(1)_{N\to\infty}.$$

The choice $N^{1/2} \ll M$ ensures that $N/M^2 \ll 1$. Thus from the above operator inequality for $\widetilde{H}_N$ and the choice of Φ_N we obtain

$$\begin{aligned}
&(1+CM^{-2})(\mu_1(\widetilde{H}_N) + N^{-1}) \geq (1+CM^{-2})\langle \Phi_N, \widetilde{H}_N \Phi_N\rangle \\
&\geq \left[\mu_1(\mathbb{H}_{\rm Bog}) - C\sqrt{\frac{M}{N}}\right]\langle \Phi_N, f_M^2 \Phi_N\rangle + \mu_1(\widetilde{H}_N)(1 - \langle \Phi_N, f_M^2 \Phi_N\rangle) - \frac{CN}{M^2} \\
&= \left[\mu_1(\mathbb{H}_{\rm Bog}) - C\sqrt{\frac{M}{N}}\right](1 + o(1)_{N\to\infty}) + \mu_1(\widetilde{H}_N) o(1)_{N\to\infty} - \frac{CN}{M^2}.
\end{aligned}$$

Using the rough information

$$|\mu_1(\mathbb{H}_{\rm Bog})| = \mathcal{O}(1), \quad |\mu_1(\widetilde{H}_N)| = \mathcal{O}(N)$$

we conclude that

$$\mu_1(\widetilde{H}_N) \geq \mu_1(\mathbb{H}_{\rm Bog}) + o(1)_{N\to\infty}.$$

This is equivalent to

$$\mu_1(H_N) \geq N e_{\rm H} + \mu_1(\mathbb{H}_{\rm Bog}) + o(1)_{N\to\infty}.$$

Step 2. Ground state energy - upper bound. We use the localization formula for the Bogoliubov Hamiltonian

$$\begin{aligned}\mathbb{H}_{\rm Bog} &\ge f_M \mathbb{H}_{\rm Bog} f_M + g_M \mathbb{H}_{\rm Bog} g_M - \frac{C}{M^2}\Big([\mathbb{H}_{\rm Bog}]_{\rm diag} + \mu_1(\mathbb{H}_{\rm Bog})\Big)\\ &\ge f_M \mathbb{H}_{\rm Bog} f_M + g_M \mathbb{H}_{\rm Bog} g_M - \frac{C}{M^2}\Big(\mathbb{H}_{\rm Bog} + C\Big).\end{aligned}$$

Using again

$$\pm f_M\Big(\widetilde{H}_N - \mathbb{H}_{\rm Bog}\Big) f_M \le C\sqrt{\frac{M}{N}} f_M(\mathbb{H}_{\rm Bog}+C) f_M$$

we have

$$f_M \mathbb{H}_{\rm Bog} f_M \ge \Big(1 + C\sqrt{\frac{M}{N}}\Big)^{-1} f_M \widetilde{H}_N f_M - C\sqrt{\frac{M}{N}}.$$

Combining with the variational principle

$$f_M \widetilde{H}_N f_M \ge f_M^2 \mu_1(\widetilde{H}_N), \quad g_M \mathbb{H}_{\rm Bog} g_M \ge g_M^2 \mu_1(\mathbb{H}_{\rm Bog})$$

we have the operator bound on Fock space $\mathcal{F}(\mathscr{H}_+)$

$$\begin{aligned}\mathbb{H}_{\rm Bog} &\ge f_M \mathbb{H}_{\rm Bog} f_M + g_M \mathbb{H}_{\rm Bog} g_M - \frac{C}{M^2}\Big(\mathbb{H}_{\rm Bog} + C\Big)\\ &\ge \Big(1 + C\sqrt{\frac{M}{N}}\Big)^{-1} f_M^2 \mu_1(\widetilde{H}_N) + g_M^2 \mu_1(\mathbb{H}_{\rm Bog}) - \frac{C}{M^2}\mathbb{H}_{\rm Bog} - C\sqrt{\frac{M}{N}}\\ &\ge\end{aligned}$$

which can be rewritten as

$$\Big(1 + CM^{-2}\Big)\mathbb{H}_{\rm Bog} \ge \Big(1 + C\sqrt{\frac{M}{N}}\Big)^{-1} f_M^2 \mu_1(\widetilde{H}_N) + g_M^2 \mu_1(\mathbb{H}_{\rm Bog}) - C\sqrt{\frac{M}{N}}$$

Now take $\Phi^{(1)}$ be the ground state for $\mathbb{H}_{\rm Bog}$. Then

$$\langle \Phi^{(1)}, \mathcal{N}_+ \Phi^{(1)}\rangle \le C < \infty.$$

By choosing

$$1 \ll M \ll N$$

we obtain

$$\langle \Phi^{(1)}, g_M^2 \Phi^{(1)}\rangle \le \langle \Phi^{(1)}, (\mathcal{N}_+/M)\Phi^{(1)}\rangle = o(1), \quad \langle \Phi^{(1)}, f_M^2 \Phi^{(1)}\rangle = 1 + o(1).$$

Thus

$$\begin{aligned}
&\Big(1+CM^{-2}\Big)\mu_1(\mathbb{H}_{\rm Bog}) = \Big(1+CM^{-2}\Big)\langle \Phi^{(1)}, \mathbb{H}_{\rm Bog}\Phi^{(1)}\rangle \\
&\ge \Big(1+C\sqrt{\frac{M}{N}}\Big)^{-1}\langle \Phi^{(1)}, f_M^2\Phi^{(1)}\rangle \mu_1(\widetilde{H}_N) + \langle \Phi^{(1)}, g_M^2\Phi^{(1)}\rangle \mu_1(\mathbb{H}_{\rm Bog}) - C\sqrt{\frac{M}{N}} \\
&= (1+o(1))\mu_1(\widetilde{H}_N) + o(1)\mu_1(\mathbb{H}_{\rm Bog}) + o(1).
\end{aligned}$$

Using the rough estimate

$$\mu_1(\mathbb{H}_{\rm Bog}) = \mathcal{O}(1), \quad \mu_1(\widetilde{H}_N) = \mathcal{O}(1)$$

we conclude that

$$\mu_1(\mathbb{H}_{\rm Bog}) \ge \mu_1(\widetilde{H}_N) + o(1).$$

This is equivalent to

$$\mu_1(H_N) \le Ne_{\rm H} + \mu_1(\mathbb{H}_{\rm Bog}) + o(1)_{N\to\infty}.$$

Combining with the lower bound in Step 1, we conclude the convergence of the ground state energy

$$\mu_1(H_N) = Ne_{\rm H} + \mu_1(\mathbb{H}_{\rm Bog}) + o(1)_{N\to\infty}.$$

Step 3: Convergence of ground state. Take any wave function $\Psi_N \in \mathscr{H}^{\otimes_s N}$ such that

$$\langle \Psi_N, H_N \Psi_N\rangle \le \mu_1(H_N) + N^{-1}, \quad \varepsilon_N := \frac{\langle \Psi_N, \mathcal{N}_+\Psi_N\rangle}{N} = o(1)_{N\to\infty}.$$

From Step 1 and Step 2, we obtain that the vector $\Phi_N = U_N\Psi_N$ satisfies

$$\frac{\langle f_M\Phi_N, \mathbb{H}_{\rm Bog} f_M \Phi_N\rangle}{\|f_M\Phi_N\|^2} \to \mu_1(\mathbb{H}_{\rm Bog}).$$

Thanks to the spectral gap $\mu_1(\mathbb{H}_{\rm Bog}) < \mu_2(\mathbb{H}_{\rm Bog})$ we conclude that up to correct choice of the phase factor,

$$\frac{f_M\Phi_N}{\|f_M\Phi_N\|} \to \Phi^{(1)}$$

strongly in Fock space $\mathcal{F}(\mathscr{H}_+)$, where $\Phi^{(1)}$ is the unique ground state for $\mathbb{H}_{\rm Bog}$. Since

$$\|g_M\Phi\| \to 0, \quad \|f_M\Phi_N\| \to 1$$

we find that $f_M\Phi_N \to \Phi^{(1)}$, and hence $\Phi_N \to \Phi^{(1)}$ strongly in Fock space $\mathcal{F}(\mathscr{H}_+)$.

Step 4: Convergence of min-max values and higher eigenstates. By the same analysis in Step 1 and Step 2, plus the min-max principle, we also obtain the convergence of all min-max values

$$\mu_i(H_N) = Ne_{\rm H} + \mu_i(\mathbb{H}_{\rm Bog}) + o(1)_{N\to\infty}, \quad \forall i = 1, 2, ...$$

In particular, this implies that for N large, H_N also have the spectral gap

$$\mu_2(H_N) - \mu_1(H_N) = \mu_2(\mathbb{H}_{\rm Bog}) - \mu_1(\mathbb{H}_{\rm Bog}) + o(1)_{N\to\infty} > 0.$$

Consequently, H_N has a unique ground state (up to a phase).
More generally, if $\mu_1(\mathbb{H}_{\rm Bog}) \le ... \le \mu_L(\mathbb{H}_{\rm Bog}) < \inf \sigma_{\rm ess}(\mathbb{H}_{\rm Bog})$, then for N large, we have

$$\mu_1(H_N) \le ... \le \mu_L(H_N) < \inf \sigma_{\rm ess}(H_N).$$

Consequently, H_N has at eigenvalues $\mu_1(H_N)$, ..., $\mu_L(H_N)$. If $\Psi_N^{(i)}$ are the corresponding eigenfunctions, then the vectors

$$\widetilde{\Psi}_N^{(i)} := \frac{f_M \Psi_N^{(i)}}{\|\Psi_N^{(i)}\|}$$

satisfy

$$\lim_{N\to\infty} \langle \widetilde{\Psi}_N^{(i)}, \widetilde{\Psi}_N^{(j)} \rangle = \delta_{i=j}, \quad \lim_{N\to\infty} \langle \widetilde{\Psi}_N^{(i)}, \mathbb{H}_{\rm Bog} \Psi_N^{(i)} \rangle = \mu_i(\mathbb{H}_{\rm Bog}).$$

By a previous exercise, this implies that up to a subsequence as $N \to \infty$, the vector $\widetilde{\Psi}_N^{(i)}$ converges strongly to an eigenvector $\Phi^{(i)}$ of $\mathbb{H}_{\rm Bog}$ with eigenvalue $\mu_i(\mathbb{H}_{\rm Bog})$. Thanks to the condensation, we have

$$\|g_M \Psi_N^{(i)}\| \to 0, \quad \|f_M \Psi_N^{(i)}\| \to 1.$$

Thus up to a subsequence as $N \to \infty$, the vector $\Psi_N^{(i)}$ converges strongly to an eigenvector $\Phi^{(i)}$ of $\mathbb{H}_{\rm Bog}$ with eigenvalue $\mu_i(\mathbb{H}_{\rm Bog})$, for all $1 \le i \le N$. This completes the proof of the theorem. *q.e.d.*