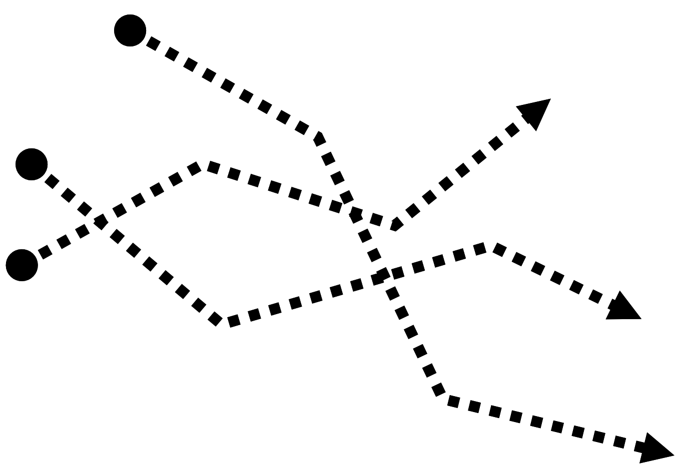
# Second quantization and lattice QFT

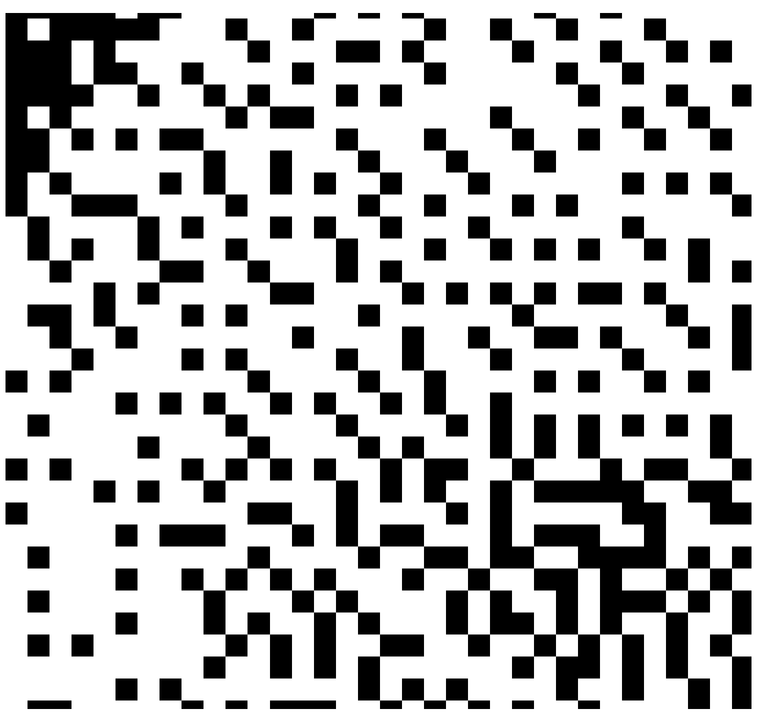
Quantum mechanics:



vector graphics (.ps)

- we follow each particle (**r** is dynamical variable)
- impractical for many electrons
- Pauli statistics causes complications (Slater det.)
- cannot capture states with fractional occupation
- Fock space is artificial construct
  'product' of Hilbert spaces of each particle

Quantum field theory:

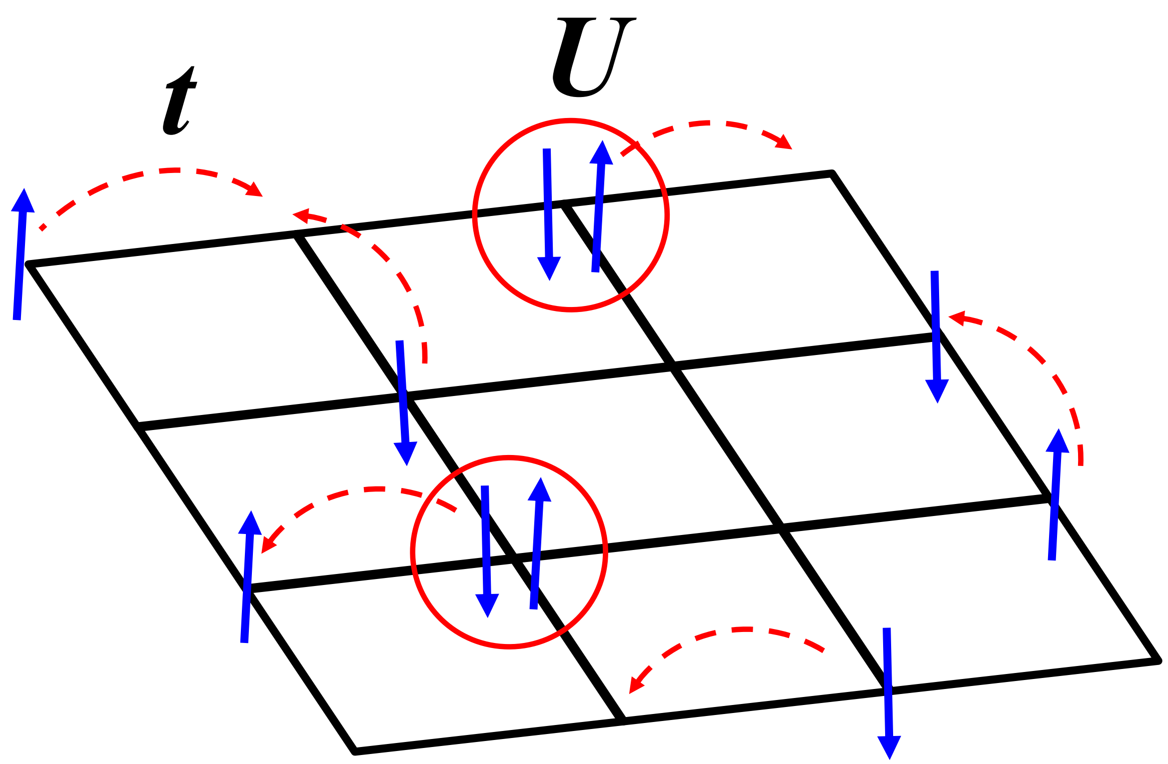


bitmap (.bmp)

- we follow the state of space points (lattice sites)
- **r** (=site index) is a parameter
- general approach
- Pauli statistics is simple (commutation rules)
- no problem with fractional occupation
- Fock space is very natural
  'product' of Hilbert spaces of lattice sites

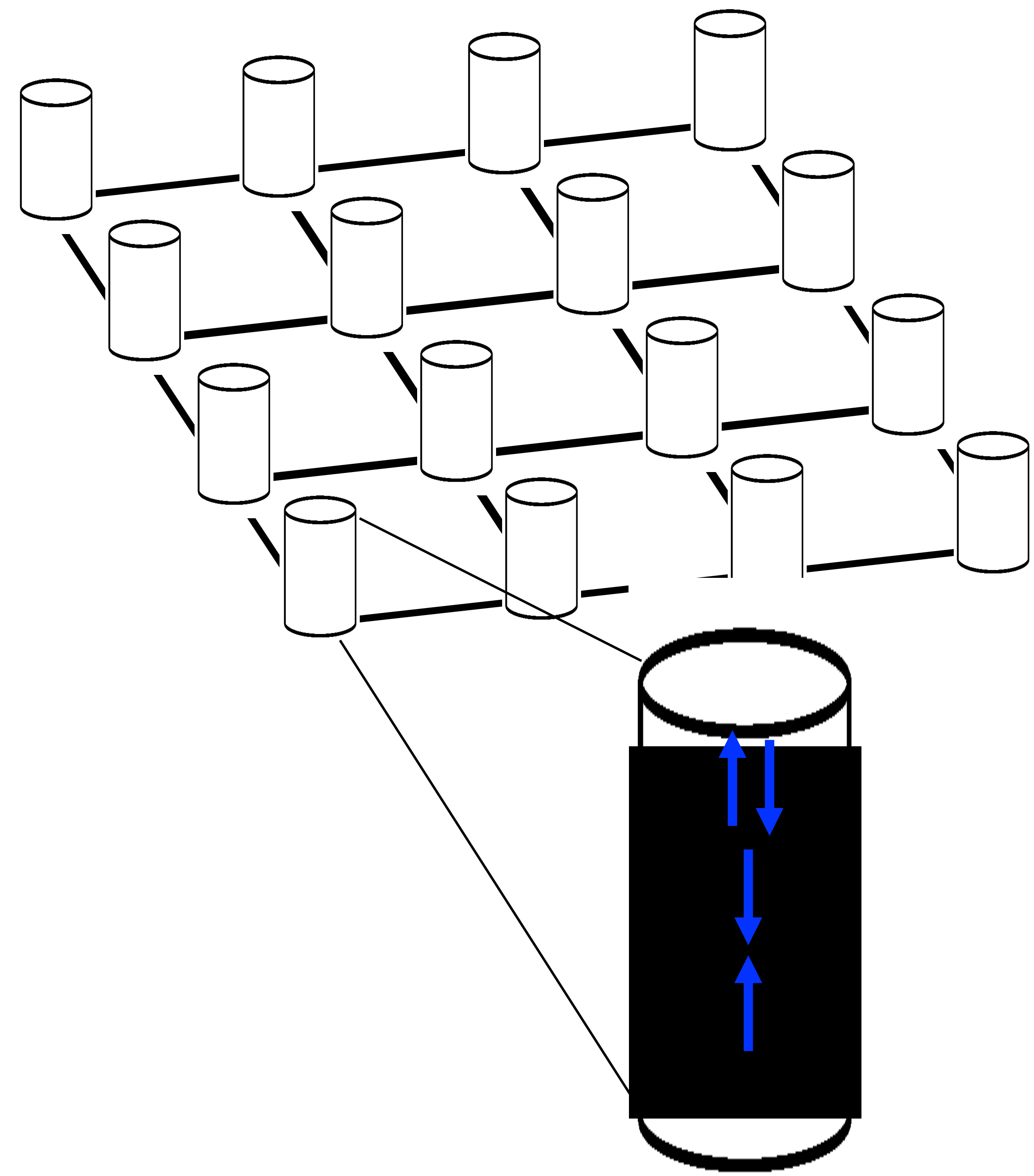
# Fock space in lattice QFT

Hubbard model




$$H = t \sum_{(ij),\sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

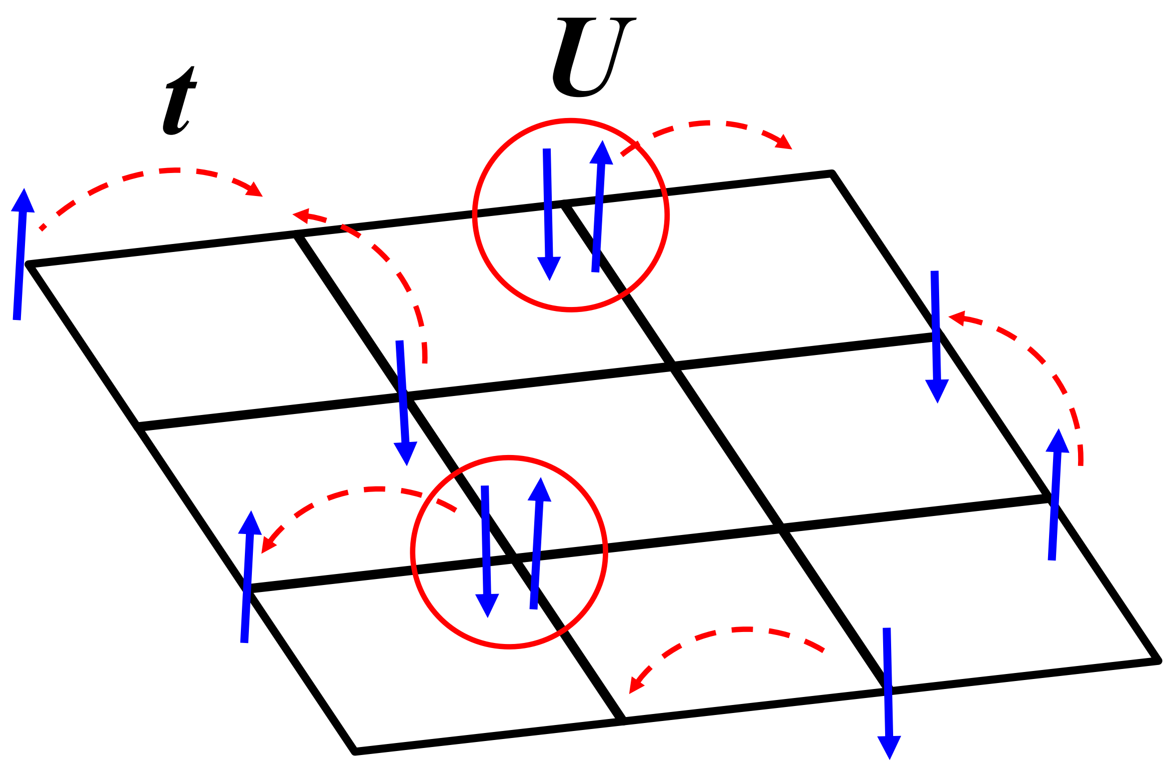
lattice Fock space



local Fock space
for fermions

# Fock space in lattice QFT

Hubbard model

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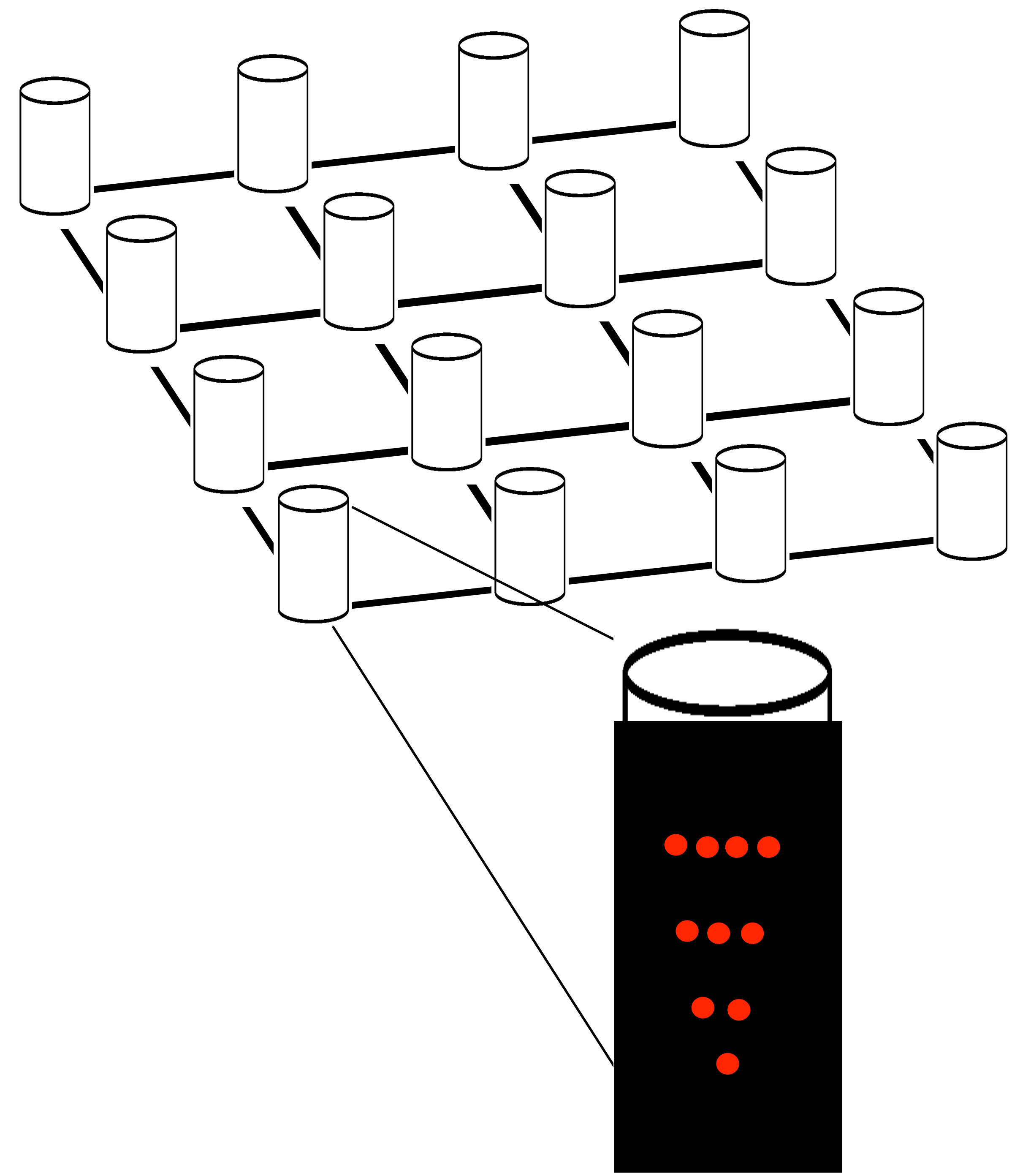
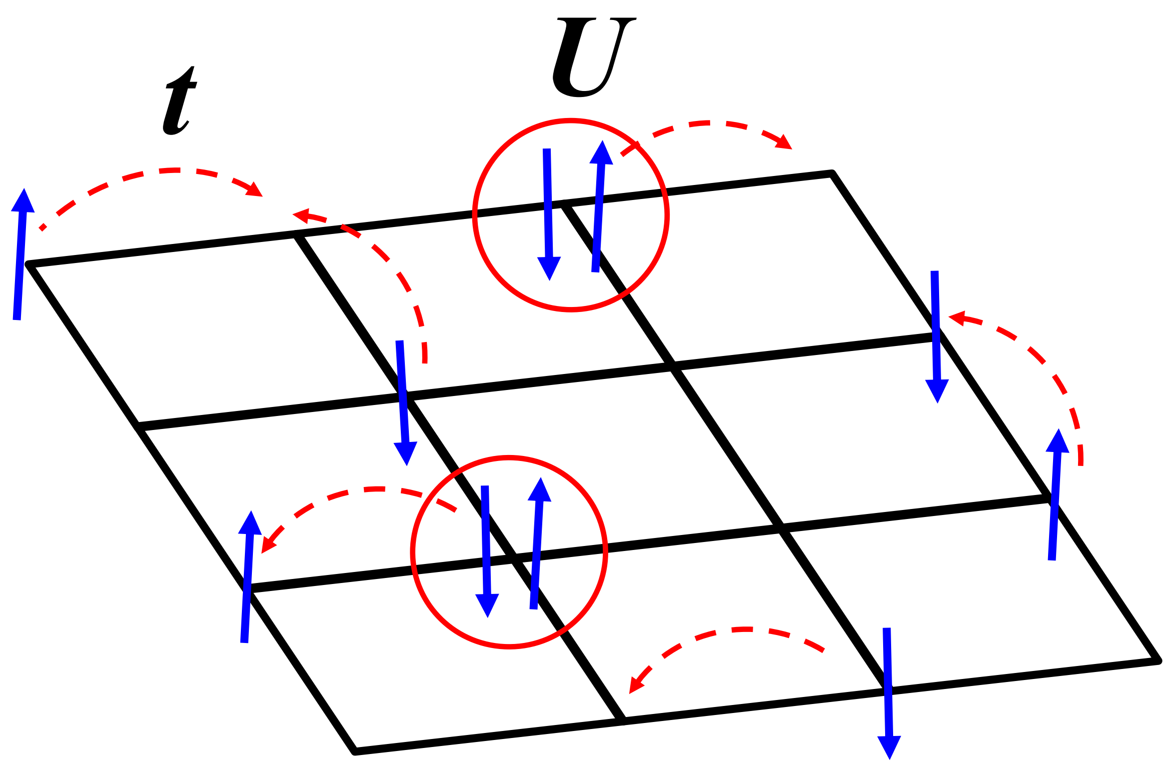
lattice Fock space



local Fock space
for bosons

# Fock space in lattice QFT

## Hubbard model




$$H = t\sum_{\langle ij\rangle,\sigma} c^\dagger_{i\sigma}c_{j\sigma} + U\sum_i n_{i\uparrow}n_{i\downarrow}$$

Definition:
Flavor = (orbital, spin)
Hilbert space of each flavor is $\{|0\rangle, |1\rangle\}$

2-flavors per site $\downarrow$ and $\uparrow$
local Fock space: $|\emptyset\rangle$

$$|\uparrow\rangle_i = c^\dagger_{i\uparrow}|\emptyset\rangle$$

$$|\downarrow\rangle_i = c^\dagger_{i\downarrow}|\emptyset\rangle$$

$$|d\rangle_i = c^\dagger_{i\uparrow}c^\dagger_{i\downarrow}|\emptyset\rangle$$

Pauli statistics:

$$\{c_i, c_j\} = c_i c_j + c_j c_i = 0$$

$$\{c_i, c^\dagger_j\} = c_i c^\dagger_j + c^\dagger_j c_i = \delta_{ij}$$

- Fock space can be constructed by acting with creation operators on vacuum
- One can use binary code to index the states
- Order of operators is crucial

# Fock space in lattice QFT

H

Density (number) operator:

$n = a^\dagger a$

$n|\emptyset\rangle = 0$

$n|1\rangle = a^\dagger a a^\dagger|\emptyset\rangle = a^\dagger|\emptyset\rangle = |1\rangle$

ite $\downarrow$ and $\uparrow$

ce: $|\emptyset\rangle$

$|\uparrow\rangle_i = c_{i\uparrow}^\dagger|\emptyset\rangle$

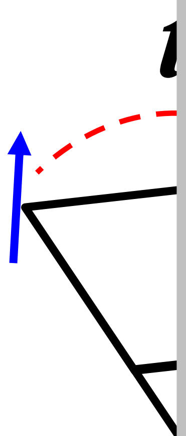
$|\downarrow\rangle_i = c_{i\downarrow}^\dagger|\emptyset\rangle$

$|d\rangle_i = c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger|\emptyset\rangle$

:

$= c_i c_j + c_j c_i = 0$

$\{c_i, c_j^\dagger\} = c_i c_j^\dagger + c_j^\dagger c_i = \delta_{ij}$



- Fock space can be constructed by acting with creation operators on vacuum
- One can use binary code to index the states
- Order of operators is crucial

$$H = t\sum_{\langle ij\rangle,\sigma} c_{i\sigma}^\dagger c_{j\sigma} + U\sum_i n_{i\uparrow}n_{i\downarrow}$$

Definition:

Flavor = (orbital, spin)

Hilbert space of each flavor is $\{|0\rangle, |1\rangle\}$

# Non-interacting problem
# Aufbau principle

$$H = \sum_{a,b} h_{ab} c_a^\dagger c_b$$

$$c_b = U_{bi} c_i, \quad (c_b^\dagger = U_{bi}^* c_i^\dagger = U_{ib}^\dagger c_i^\dagger) \qquad \{c_i, c_j^\dagger\} = U_{ia}^\dagger \{c_a, c_b^\dagger\} U_{bj} = U_{ia}^\dagger \delta_{ab} U_{bj} = \delta_{ij}$$

$$H = \sum_i \epsilon_i c_i^\dagger c_i$$

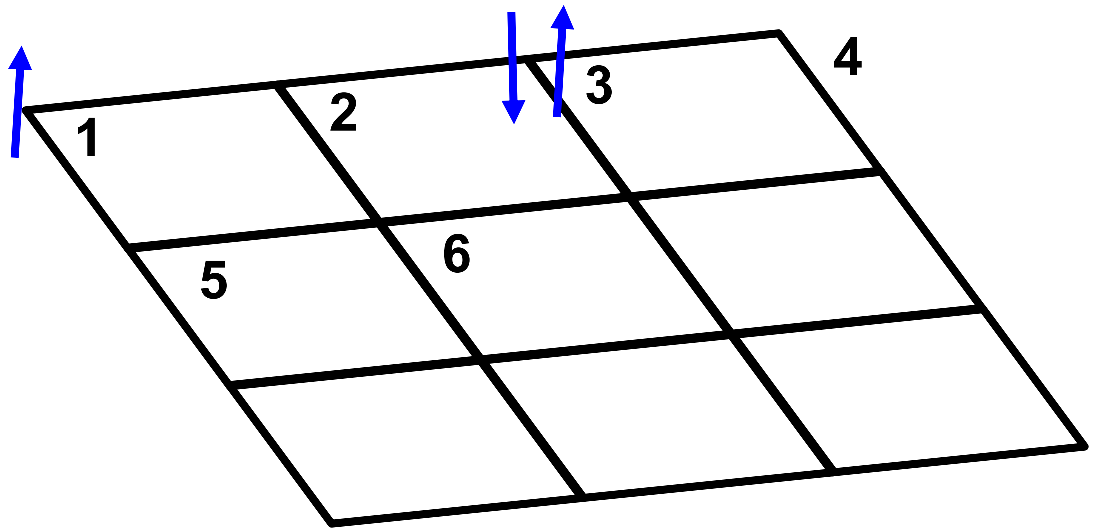
Canonical commutation relations!

$$|\phi\rangle = c_{i_1}^\dagger \dots c_{i_N}^\dagger |\mathrm{vac}\rangle$$

$$H|\phi\rangle = \left( \sum_{k=1}^{N} \epsilon_{i_k} \right) |\phi\rangle$$

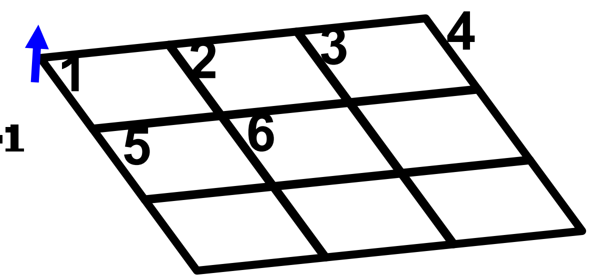
# Example of wave functions

$c_{3\uparrow}^{\dagger} c_{3\downarrow}^{\dagger} c_{1\uparrow}^{\dagger} |\mathrm{vac}\rangle$

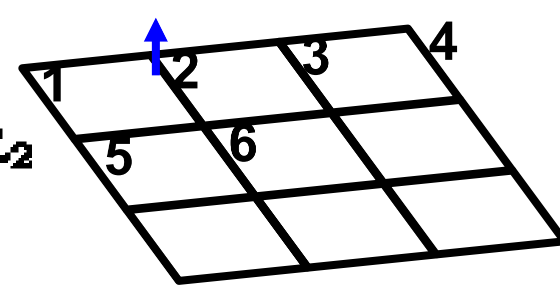



$$c_{\mathbf{k}\uparrow}^{\dagger} |\mathrm{vac}\rangle = \frac{1}{\sqrt{N}} \sum_i e^{i\mathbf{k}\cdot\mathbf{R}_i} c_{i\uparrow}^{\dagger} |\mathrm{vac}\rangle$$

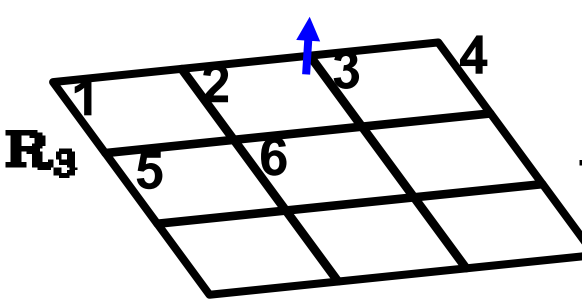
$e^{i\mathbf{k}\cdot\mathbf{R}_1}$




$+e^{i\mathbf{k}\cdot\mathbf{R}_2}$

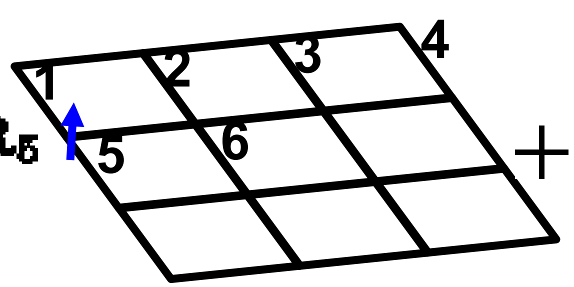



$+e^{i\mathbf{k}\cdot\mathbf{R}_3}$




$+\cdots$

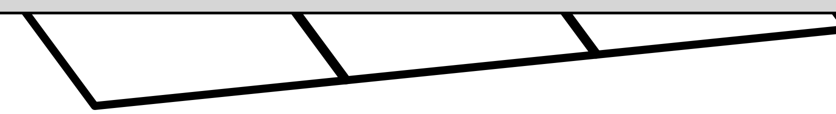
$+e^{i\mathbf{k}\cdot\mathbf{R}_5}$




$+\cdots$

- Total size of fermionic Fock space is $4^N$. (bosonic is infinite)
- Any state can be written as a linear combination of the states in occupation number basis

$|\phi\rangle = c^\dagger_{3\uparrow}c^\dagger_{3\downarrow}$



## Meaning of the Hamiltonian:

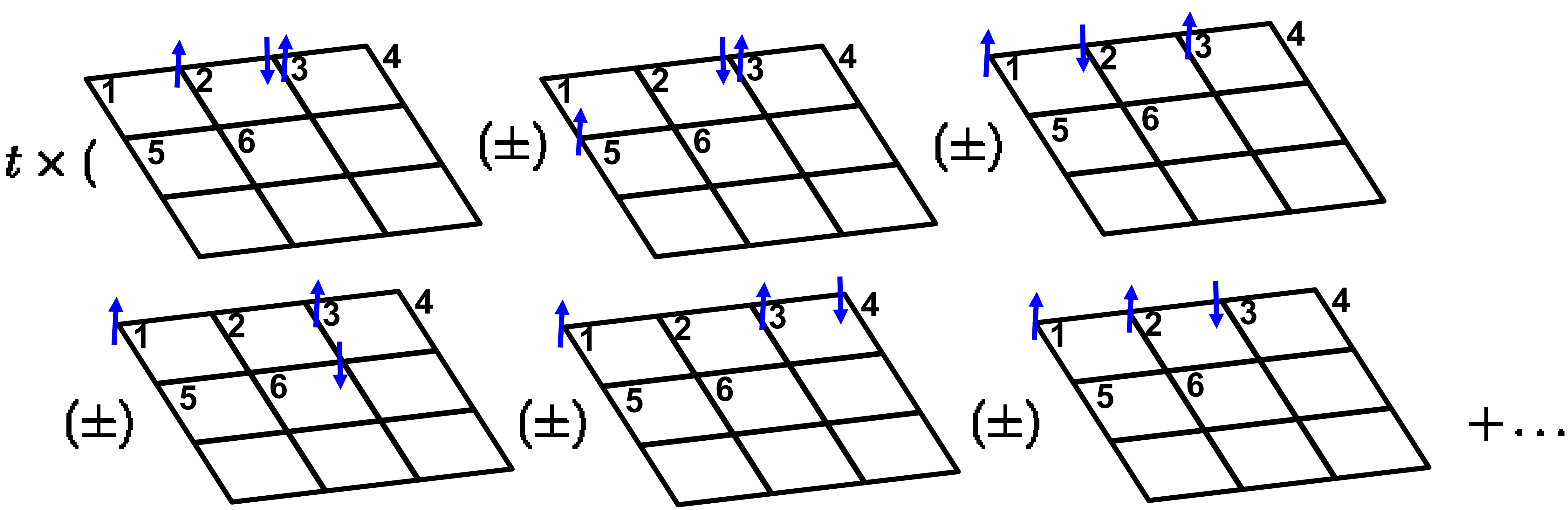
$$U(t) = e^{-itH} = (e^{-i\frac{t}{n}H})^n \approx (I - i\frac{t}{n}H)^n$$

Hamiltonian generates the time evolution of the system!

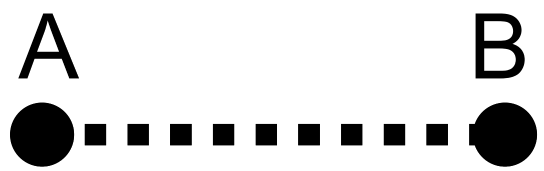
[redacted]

- Move annihilation operators to the right ->calculate number of (anti)commutators
- Put creations operators to standard order (for fermions only)-> determine signs

$H|\phi\rangle =$



# Hubbard molecule

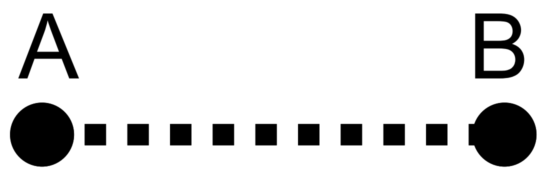



$$H = t(a_\uparrow^\dagger b_\uparrow + a_\downarrow^\dagger b_\downarrow + b_\uparrow^\dagger a_\uparrow + b_\downarrow^\dagger a_\downarrow) + U(a_\uparrow^\dagger a_\downarrow^\dagger a_\downarrow a_\uparrow + b_\uparrow^\dagger b_\downarrow^\dagger b_\downarrow b_\uparrow)$$

Remarks:

- number of 1-p states N=4
- dimension of the Fock space $2^N = 16$
- dimension of an M-particle sector $\binom{N}{M}$, e.g., $\binom{4}{2} = 6$
- density/particle number operator $n_c = c^\dagger c$

# Hubbard molecule




$$H = t(a_\uparrow^\dagger b_\uparrow + a_\downarrow^\dagger b_\downarrow + b_\uparrow^\dagger a_\uparrow + b_\downarrow^\dagger a_\downarrow) + U(a_\uparrow^\dagger a_\downarrow^\dagger a_\downarrow a_\uparrow + b_\uparrow^\dagger b_\downarrow^\dagger b_\downarrow b_\uparrow)$$

Construction of the Hamiltonian (in occupation number basis):

- sign convention, e.g. $c_{i_3}^\dagger c_{i_2}^\dagger c_{i_1}^\dagger |\emptyset\rangle,\ i_3 > i_2 > i_1$
- order the 1-p states: $\{b\uparrow, b\downarrow, a\uparrow, a\downarrow\}$

Two options: Construct the matrices of the elementary creation/anihilation operators. (computer - sparse matrices)

Construct the basis states and compute the matrix elements of *H* using commutation relations. (pen&paper)

# Hubbard molecule

$$H = t(a_\uparrow^\dagger b_\uparrow + a_\downarrow^\dagger b_\downarrow + b_\uparrow^\dagger a_\uparrow + b_\downarrow^\dagger a_\downarrow) + U(a_\uparrow^\dagger a_\downarrow^\dagger a_\downarrow a_\uparrow + b_\uparrow^\dagger b_\downarrow^\dagger b_\downarrow b_\uparrow)$$

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- order the 1-p states: $\{b\uparrow, b\downarrow, a\uparrow, a\downarrow\}$

Let us focus on the 2 electron sector (the rest is trivial)

The basis:

| index | $i_2 i_1$ | state |
|---|---|---|
| 1 | 21 | $a_\uparrow^\dagger a_\downarrow^\dagger \vert\emptyset\rangle$ |
| 2 | 31 | $b_\downarrow^\dagger a_\downarrow^\dagger \vert\emptyset\rangle$ |
| 3 | 41 | $b_\uparrow^\dagger a_\downarrow^\dagger \vert\emptyset\rangle$ |
| 4 | 32 | $b_\downarrow^\dagger a_\uparrow^\dagger \vert\emptyset\rangle$ |
| 5 | 42 | $b_\uparrow^\dagger a_\uparrow^\dagger \vert\emptyset\rangle$ |
| 6 | 43 | $b_\uparrow^\dagger b_\downarrow^\dagger \vert\emptyset\rangle$ |

Hamiltonian:

$$H = \begin{pmatrix} U & 0 & t & -t & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ t & 0 & 0 & 0 & 0 & t \\ -t & 0 & 0 & 0 & 0 & -t \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & t & -t & 0 & U \end{pmatrix}$$

# Hubbard molecule

$$H = t(a_\uparrow^\dagger b_\uparrow + a_\downarrow^\dagger b_\downarrow + b_\uparrow^\dagger a_\uparrow + b_\downarrow^\dagger a_\downarrow) + U(a_\uparrow^\dagger a_\downarrow^\dagger a_\downarrow a_\uparrow + b_\uparrow^\dagger b_\downarrow^\dagger b_\downarrow b_\uparrow)$$

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Hamiltonian:

$$H = \begin{pmatrix} U & 0 & t & -t & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ t & 0 & 0 & 0 & 0 & t \\ -t & 0 & 0 & 0 & 0 & -t \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & t & -t & 0 & U \end{pmatrix}$$

Spectrum:

| Energy | Eigenfunctions | Total spin |
|---|---|---|
| $0$ | $\lvert 2\rangle$ , $\lvert 5\rangle$, $\frac{1}{\sqrt{2}}(\lvert 3\rangle + \lvert 4\rangle)$ | $(S=1)$ |
| $U$ | $\frac{1}{\sqrt{2}}(\lvert 1\rangle - \lvert 6\rangle)$ | $(S=0)$ |
| Ground state: $\frac{1}{2}(U - \sqrt{U^2+16t^2})$ | $\approx \frac{1}{\sqrt{2}}(-\lvert 3\rangle + \lvert 4\rangle)$ | $(S=0)$ |
| $\frac{1}{2}(U + \sqrt{U^2+16t^2})$ | $\approx \frac{1}{\sqrt{2}}(\lvert 1\rangle + \lvert 6\rangle)$ | $(S=0)$ |

# Hubbard molecule

Various operators:

| | | |
|---|---|---|
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$$n_a = \begin{pmatrix} 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

$a_\uparrow^\dagger a_\uparrow + a_\downarrow^\dagger a_\downarrow$

$$S_a^x = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad S_a^y = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{i}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{i}{2} & 0 \\ 0 & -\frac{i}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{i}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad S_a^z = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

$a_\downarrow^\dagger a_\uparrow + a_\uparrow^\dagger a_\downarrow$

$i(a_\downarrow^\dagger a_\uparrow - a_\uparrow^\dagger a_\downarrow)$

$a_\uparrow^\dagger a_\uparrow - a_\downarrow^\dagger a_\downarrow$

# Hubbard molecule

Various operators:

1 21 $a_\uparrow^\dagger a_\downarrow^\dagger|\emptyset\rangle$

2 31 $b_\downarrow^\dagger a_\downarrow^\dagger|\emptyset\rangle$

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$$a_\uparrow^\dagger a_\uparrow + a_\downarrow^\dagger a_\downarrow$$

$$S^x = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & \frac{1}{2} & 0 \\ 0 & \frac{1}{2} & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad S^y = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{i}{2} & \frac{i}{2} & 0 & 0 \\ 0 & -\frac{i}{2} & 0 & 0 & \frac{i}{2} & 0 \\ 0 & -\frac{i}{2} & 0 & 0 & \frac{i}{2} & 0 \\ 0 & 0 & -\frac{i}{2} & -\frac{i}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad S^z = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

$$S^x = S_a^x + S_b^x \qquad S^y = S_a^y + S_b^y \qquad S^z = S_a^z + S_b^z$$

# Some expectation values

Ground state:

$$|\mathrm{GS}> = \frac{1}{\sqrt{2+\mu^2}}\begin{pmatrix}1\\0\\-\mu\\\mu\\0\\1\end{pmatrix}; \quad \mu = \frac{1}{4}(u+\sqrt{u^2+16})$$

Lowest excitation energy: $$E_1 = \frac{1}{2}(\sqrt{16+u^2}-u) \approx \frac{4}{u}$$

Total spin (conserved): $$\langle \mathrm{GS}|S^2|\mathrm{GS}\rangle = 0$$

*large u=U/t*

Spin per atom (non-conserved): $$\langle \mathrm{GS}|S_a^2|\mathrm{GS}\rangle = \frac{3}{4} - \frac{3}{8}\frac{16}{u^2+u\sqrt{u^2+16}+16}$$

$$\approx \frac{3}{4}(1-\frac{4}{u^2})$$

# Some physics

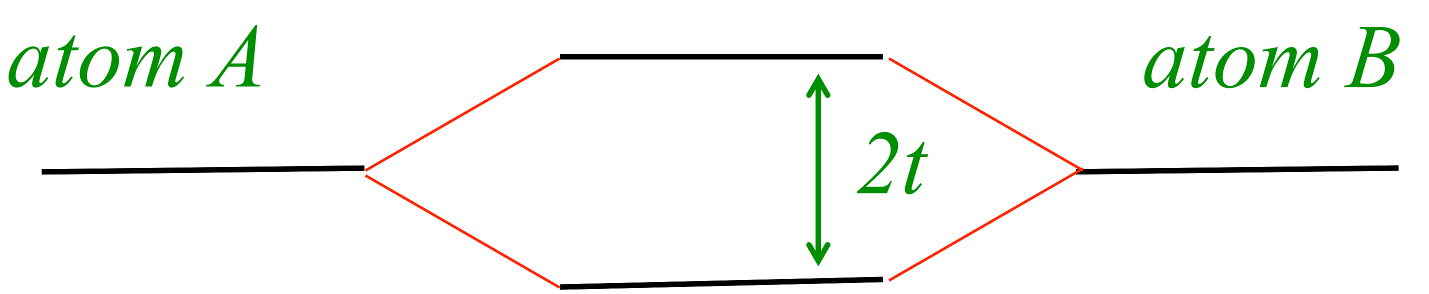
G

$$|GS> = \frac{1}{\sqrt{2+\mu^2}} \begin{pmatrix} 1 \\ 0 \\ -\mu \\ \mu \\ 0 \\ 1 \end{pmatrix}; \quad \mu = \frac{1}{4}\left(u + \sqrt{u^2+16}\right)$$

Non-interacting limit (μ=1):

$$|GS\rangle = \frac{1}{2}\left(a_\uparrow^\dagger a_\downarrow^\dagger - b_\uparrow^\dagger a_\downarrow^\dagger + b_\downarrow^\dagger a_\uparrow^\dagger + b_\uparrow^\dagger b_\downarrow^\dagger\right)|\emptyset\rangle$$

Bonding—anti-bonding picture:



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$$= \frac{1}{2}\left(a_\uparrow^\dagger - b_\uparrow^\dagger\right)\left(a_\downarrow^\dagger - b_\downarrow^\dagger\right)|\emptyset\rangle$$

Bonding—anti-bonding picture: