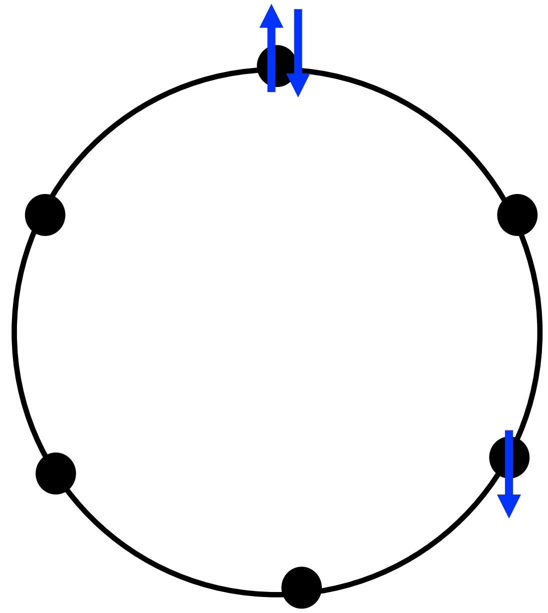
6-site Hubbard model

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

Large Fock space: dim 2^{12}

Use conservation of S_z : (s1, s2) sectors of dim $\binom{6}{s_1}\binom{6}{s_2}$

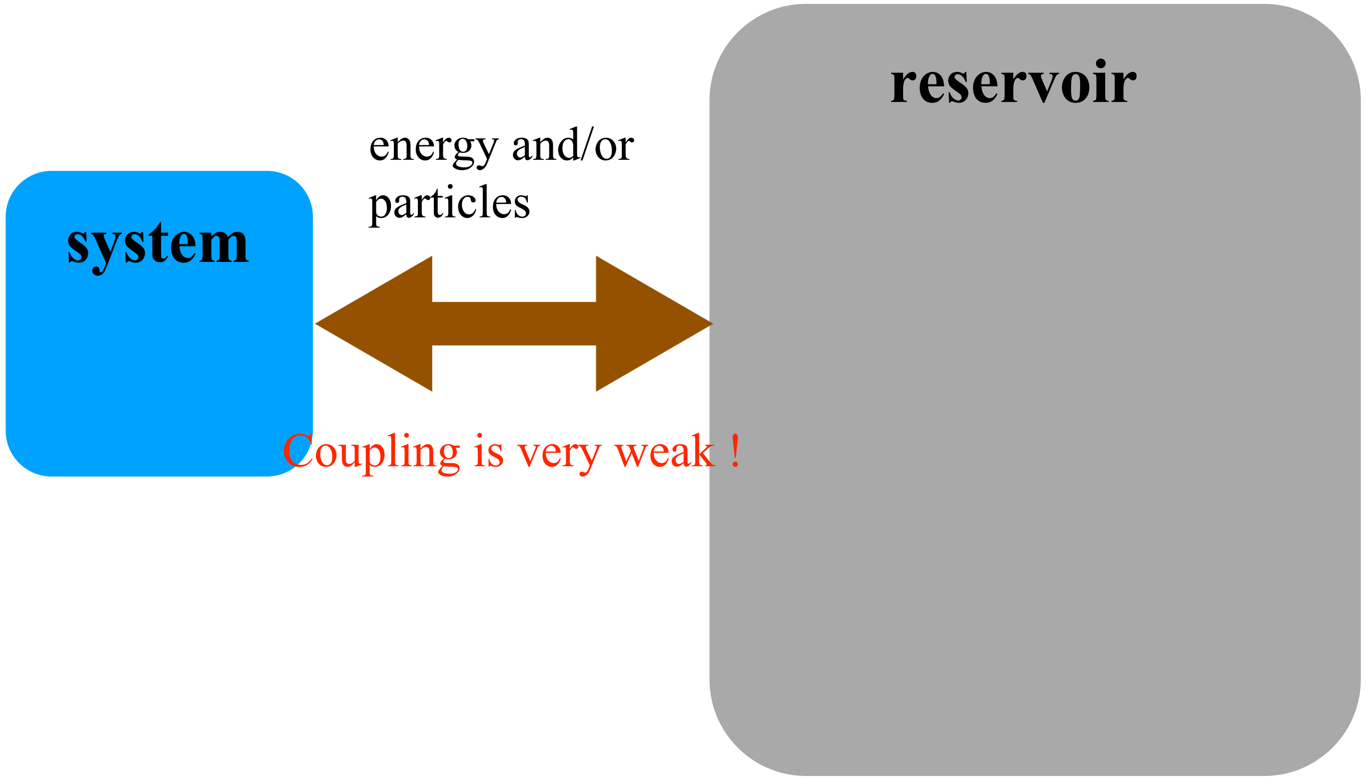
We study all sectors with N=6 simultaneously (6,0), (5, 1), (4,2), (3,3), (2,4), (1,5), (0,6)



Thermal equilibrium

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

Thermal averages (finite temperature):



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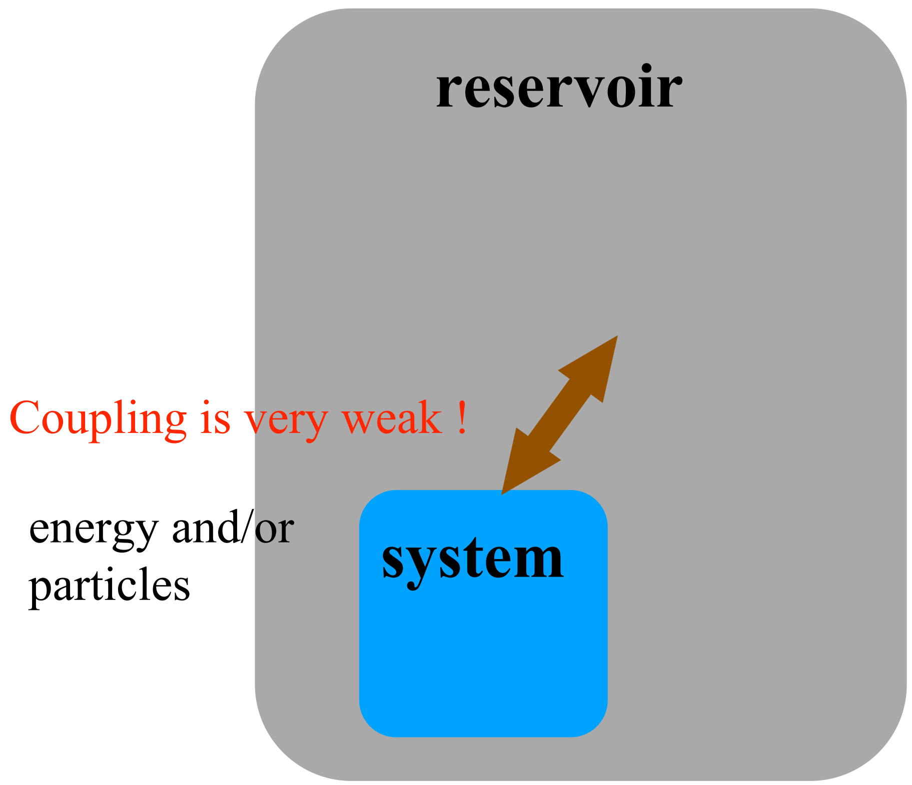
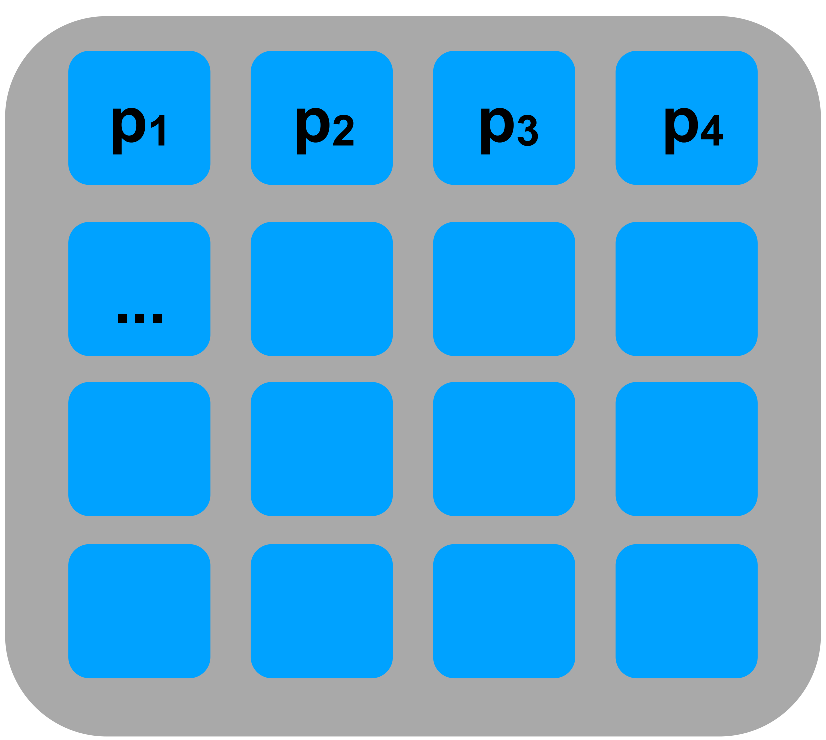


Thermal equilibrium

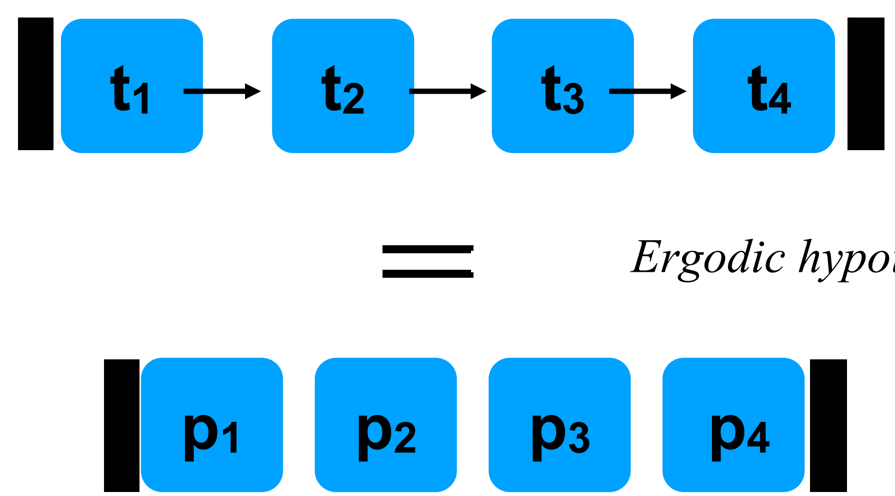
$$H = t \sum_{(ij),\sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

ensemble averaging:

Measurement involves different (weakly coupled) parts of the system, e.g., total moment is a sum of local moments



Measurement involves averaging over (long) time (=duration of measurement)



Ergodic hypothesis

Averaging over various realizations of the system

Thermal equilibrium

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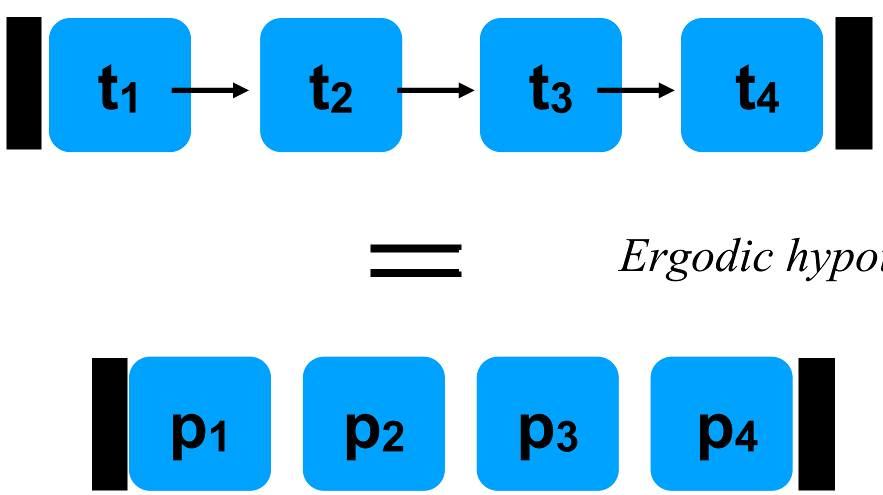

Ergodic hypothesis

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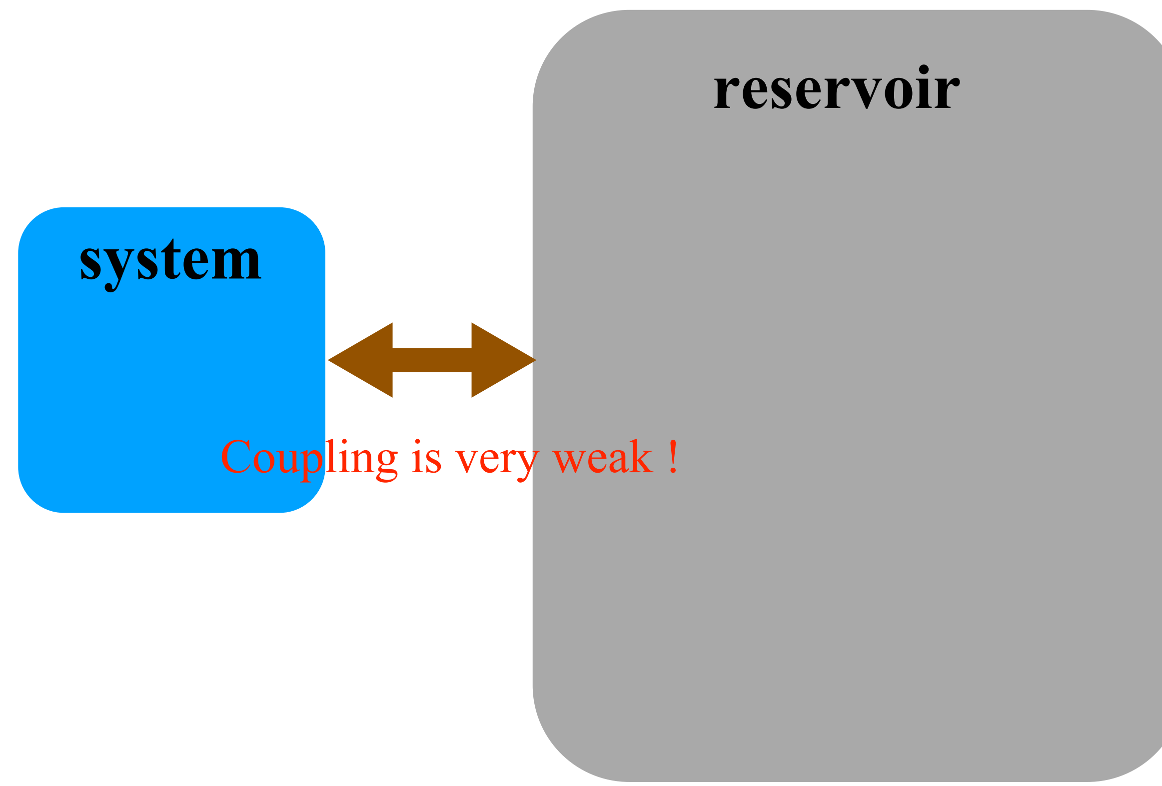
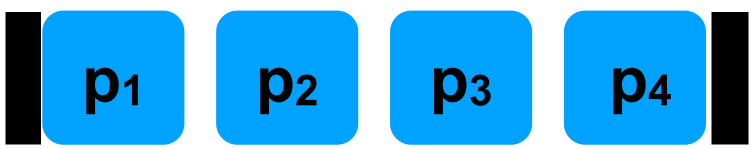


The slow dynamics due to system-reservoir interaction is replaced by ensemble averaging (the fast dynamics of the system itself is retained)

Thermal equilibrium

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

ensemble averaging:



Averaging over various realizations of the system

How do we get the probabilities?

Statistical considerations => in thermal equilibrium:

$$\langle\langle O \rangle\rangle_T = \frac{1}{Z(T)} \sum_l \langle l | O | l \rangle \exp(-\frac{E_l}{k_B T})$$

$$Z(T) = \sum_l \exp(-\frac{E_l}{k_B T})$$

avg. at temperature T

sum over eigenstates l

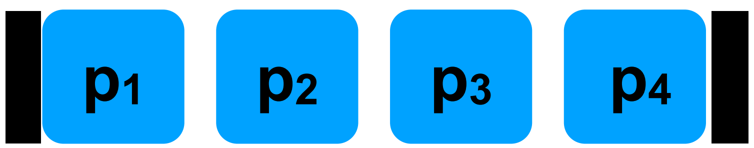
Boltzmann weight/factor

Partition function

Thermal equilibrium

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

ensemble averaging:



Averaging over various realizations of the system

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$$\rho = \frac{1}{Z} \exp(-\beta H) \qquad Z = \mathrm{Tr}\exp(-\beta H) \qquad \beta = \frac{1}{k_B T}$$

density matrix (statistical operator)

Hamiltonian (operator)

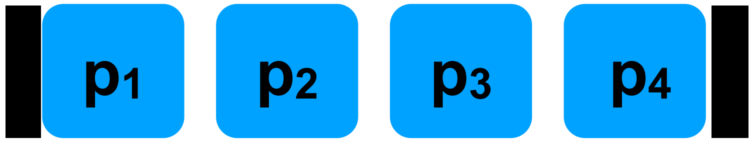
(number)

inverse temperature

Thermal equilibrium

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

ensemble averaging:



Averaging over various realizations of the system

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Ground state:

$G_{AB}(t) =$ [redacted]

Finite temperature:

$$= \frac{1}{Z} \mathrm{Tr}(e^{-\beta H} e^{itH} A e^{-itH} B)$$

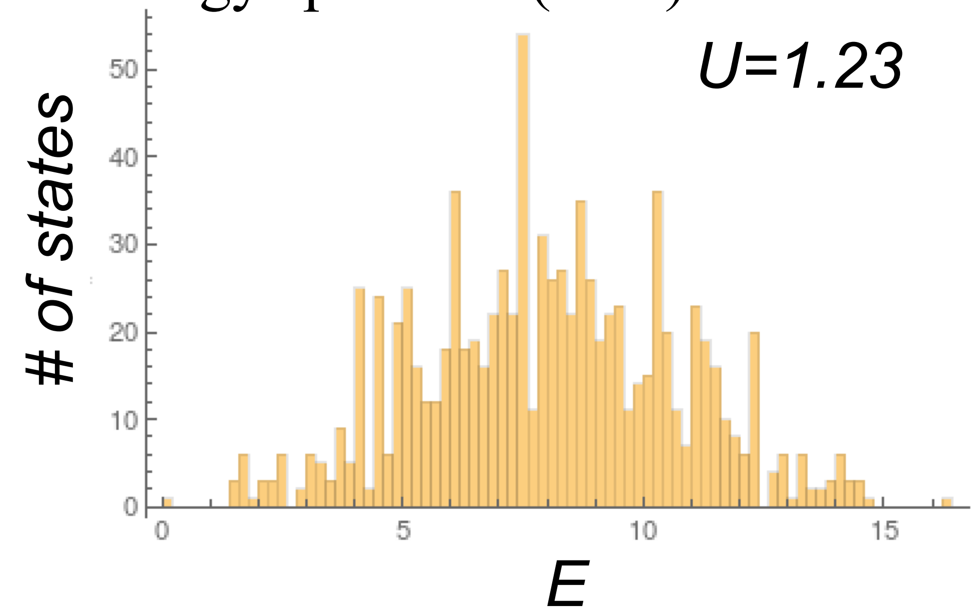
$$= \frac{1}{Z} \sum_{n,m} \langle m | e^{-\beta H} e^{itH} A | n \rangle \langle n | e^{-itH} B | m \rangle$$

$$= \frac{1}{Z} \sum_{n,m} e^{-\beta E_m} e^{-it(E_n - E_m)} \langle m | A | n \rangle \langle n | B | m \rangle$$

Thermodynamic observables

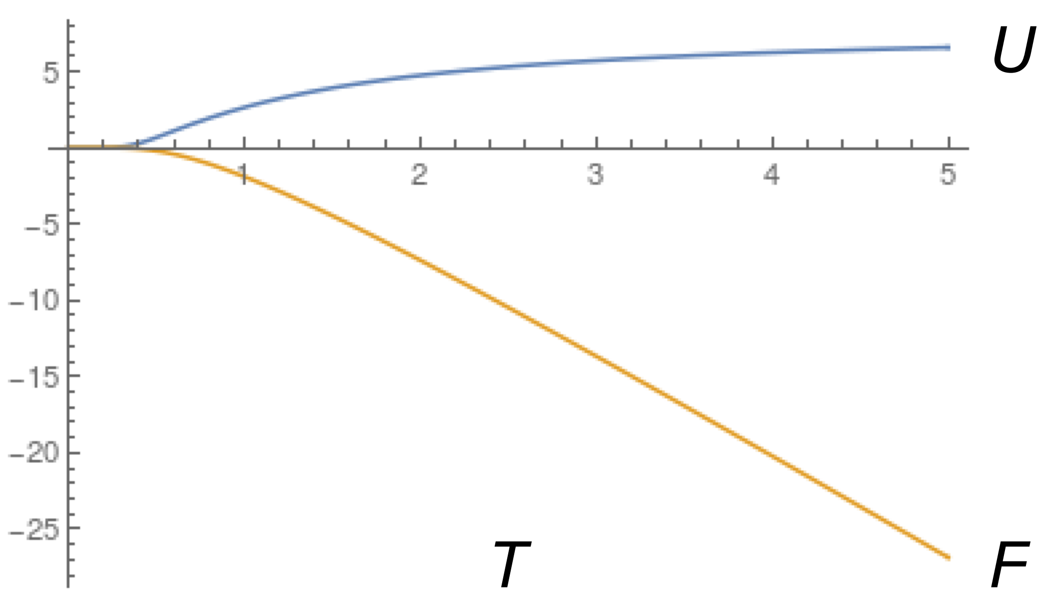
$$H = t \sum_{\langle ij \rangle, \sigma} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

Energy spectrum (N=6)



Thermodynamic observables:

$U = \langle\langle H \rangle\rangle$	internal energy
$F = -T \ln Z(T)$	free energy
$F = U - TS$	entropy S
$c = \frac{\partial U}{\partial T}$	specific heat (heat capacity)



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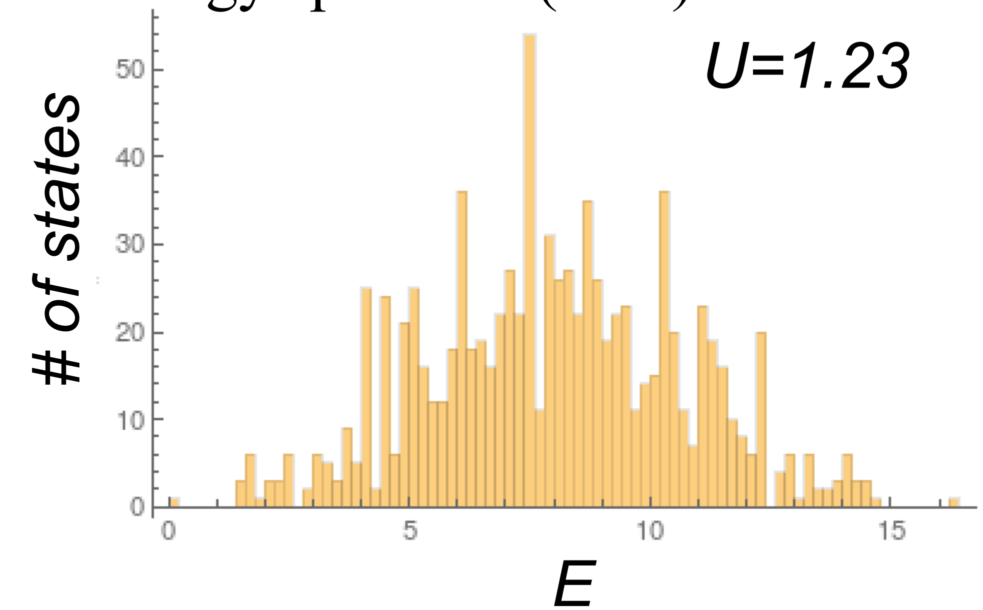

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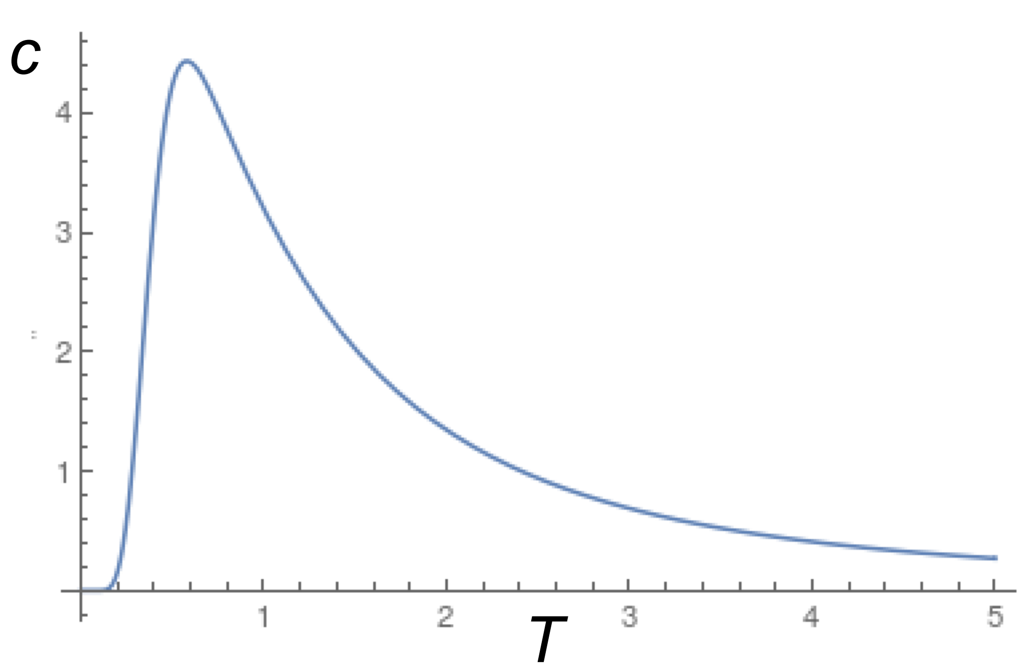
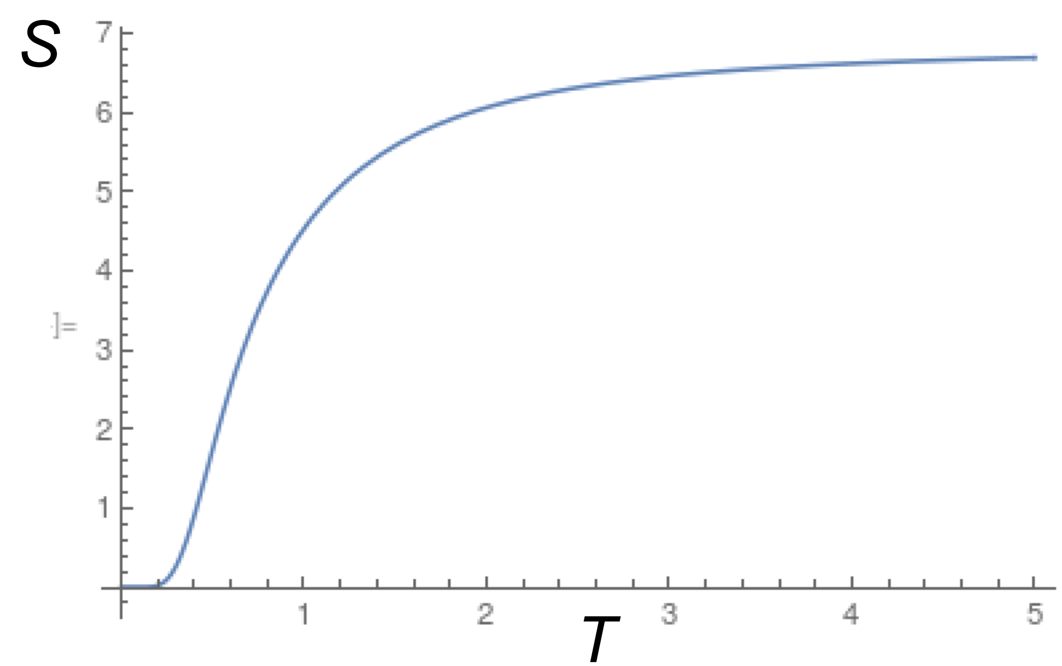
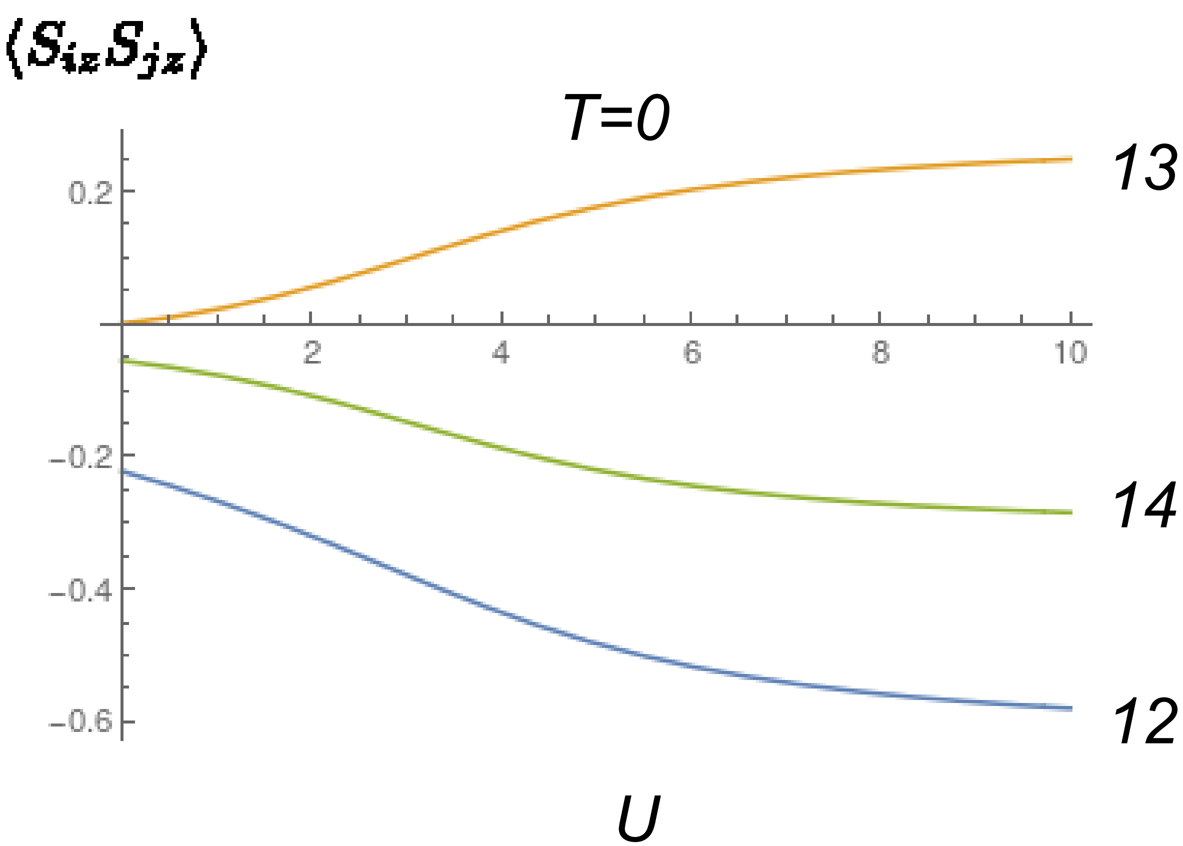


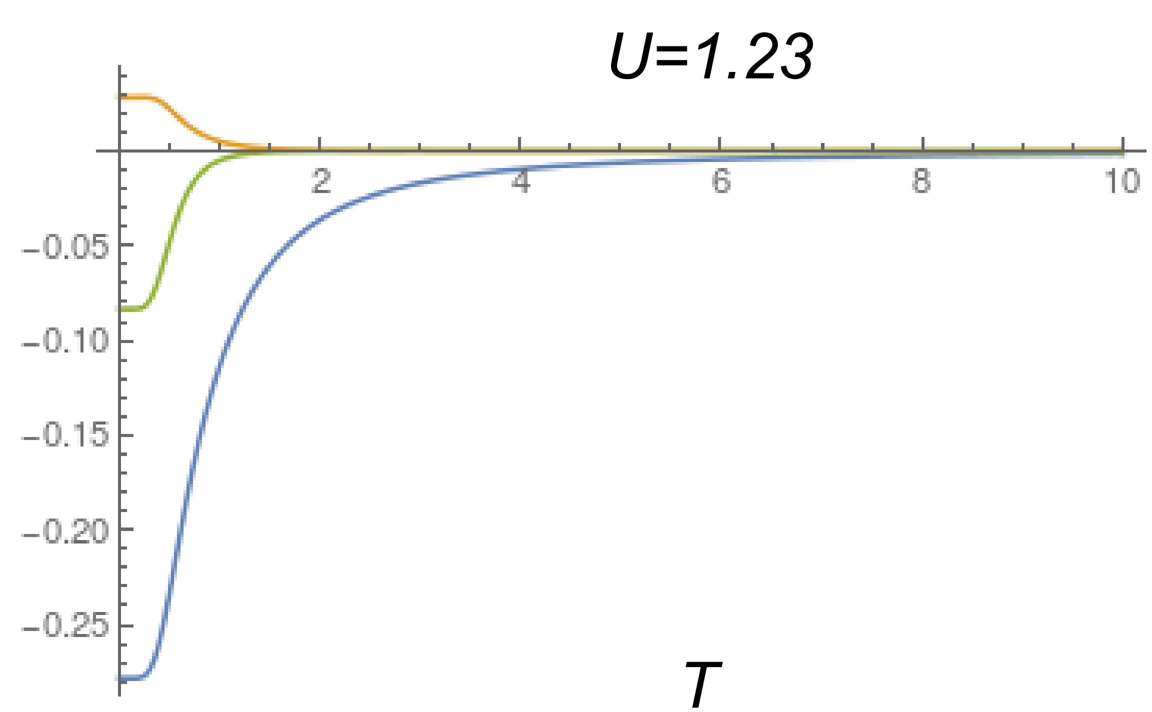


Correlation functions

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

Expectation values/correlation functions:



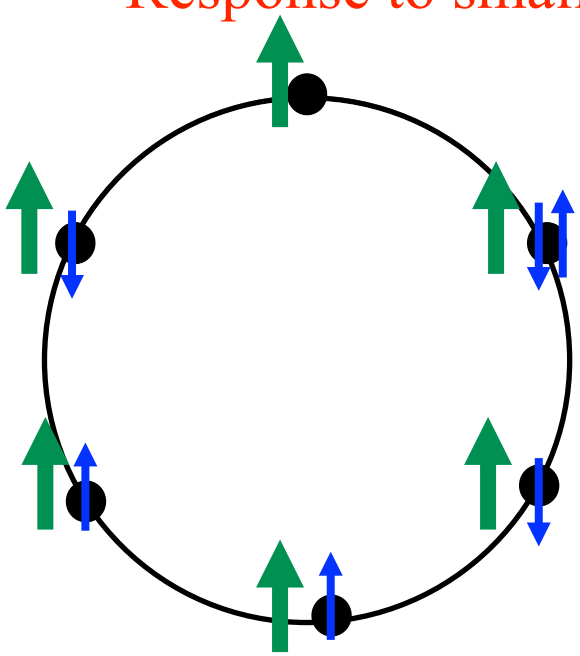


Linear response

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

Why correlation functions?

- Contributions to interaction energy of the system $\langle n_{i\uparrow} n_{i\downarrow} \rangle$
- Response to small perturbations



external uniform field

$$\delta \langle\langle S_z \rangle\rangle = \chi \cdot \delta h$$

$$\langle\langle S_z \rangle\rangle_T = \frac{1}{Z(h)} \sum_l S_z(l) \exp(-\frac{E_l - h S_z(l)}{T}) \equiv \frac{S(h)}{Z(h)}$$

$$S_z(l) = \langle l | S_z | l \rangle$$

$$\frac{\partial Z(h)}{\partial h} = \frac{S(h)}{T}$$

$$\left.\frac{\partial \langle\langle S_z \rangle\rangle}{\partial h}\right|_{h=0} = -\left.\frac{S^2(h)}{T Z^2(h)}\right|_{h=0} + \left.\frac{1}{Z(h)} \frac{\partial S(h)}{\partial h}\right|_{h=0}$$

$$= \frac{\langle\langle S_z^2 \rangle\rangle}{T}$$

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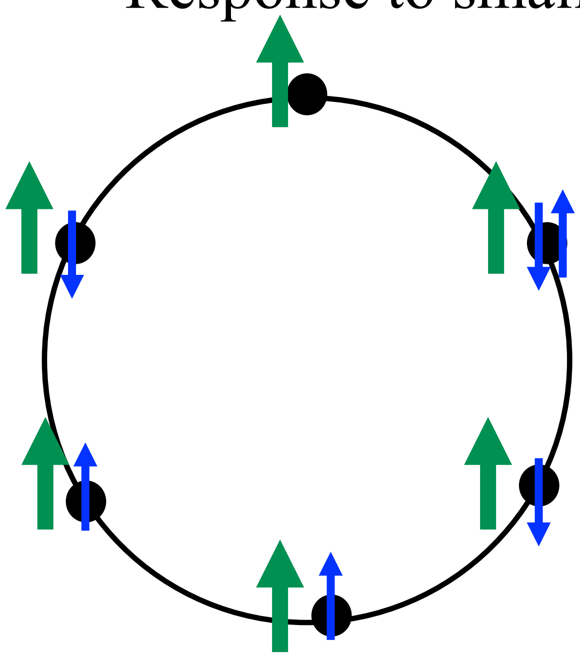

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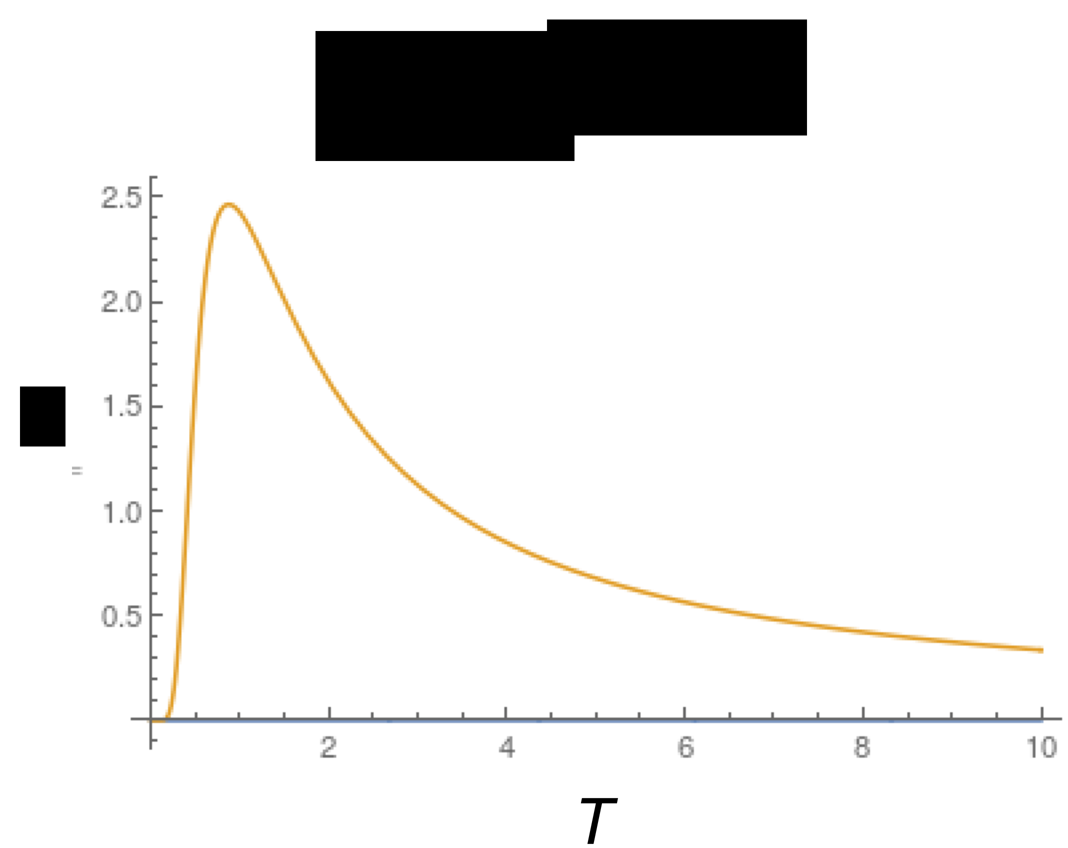
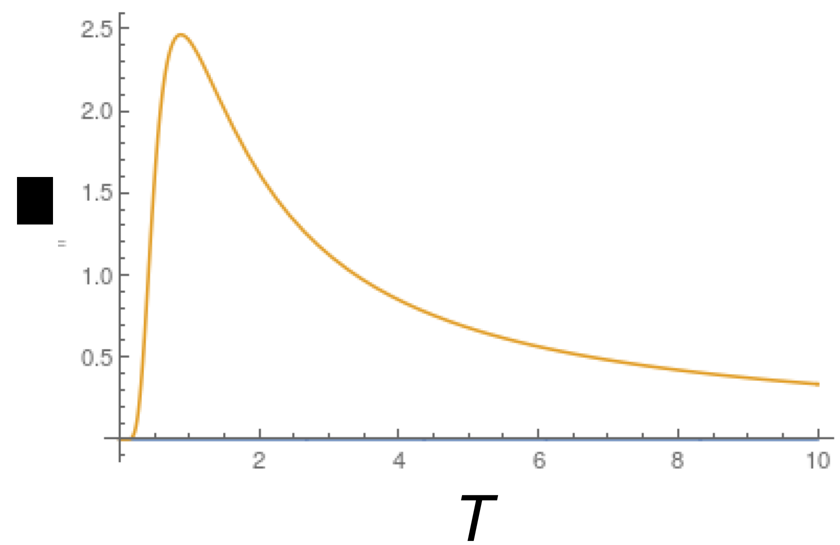


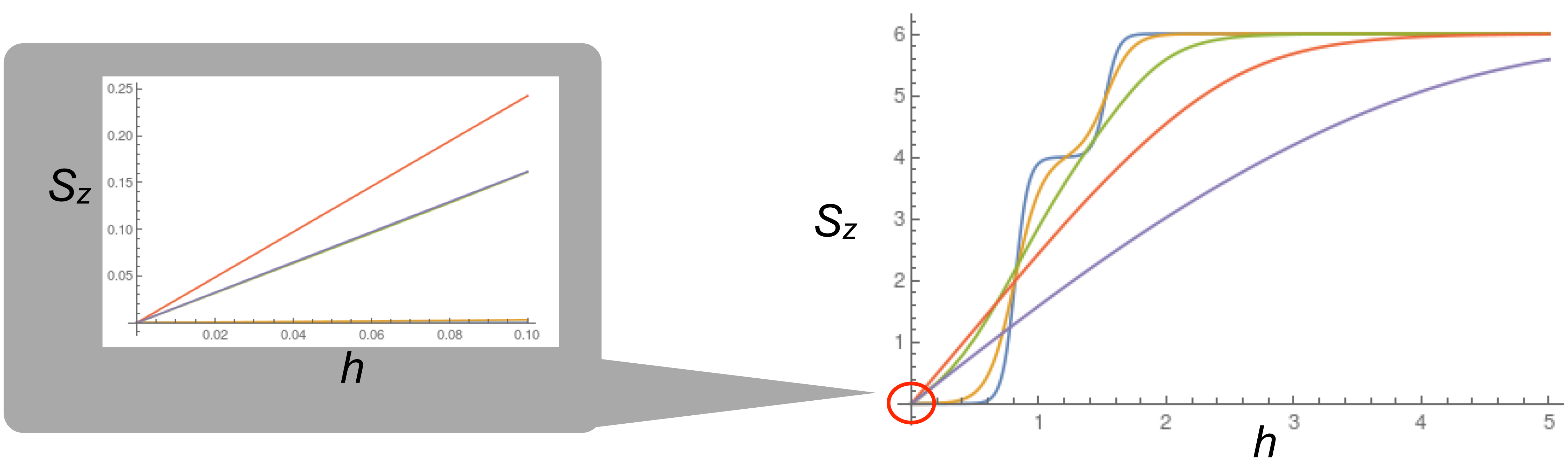
Linear response

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

Does it work?
Let's calculate a response to finite h.

$$\delta\langle\langle S_z\rangle\rangle = \chi\cdot\delta h$$





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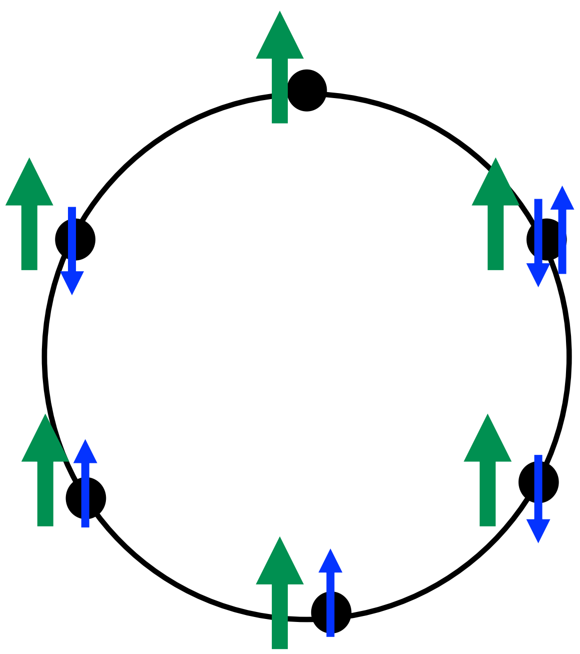


external uniform field

$$\delta\langle\langle S_z\rangle\rangle = \chi\cdot\delta h$$

Uniform susceptibility is a special case because $[S_z, H] = 0$

General case (e.g. local susceptibility):

$$\chi_{\mathrm{loc}}(\omega) = -\langle[S_{iz}(t), S_{iz}(0)]\rangle_\omega = \langle S_{iz}S_{iz}\rangle_{-\omega} - \langle S_{iz}S_{iz}\rangle_\omega$$

Linear response (perturbative) regime

Kubo formula

$H = H_0 + V(t)$

External time-dependent field (el.-mag. field, photon)

[redacted]

Initial state (ground state)

Evolution operator

H_0 and V do not commute and thus is it not possible to split the exponential even if V did not depend on time!

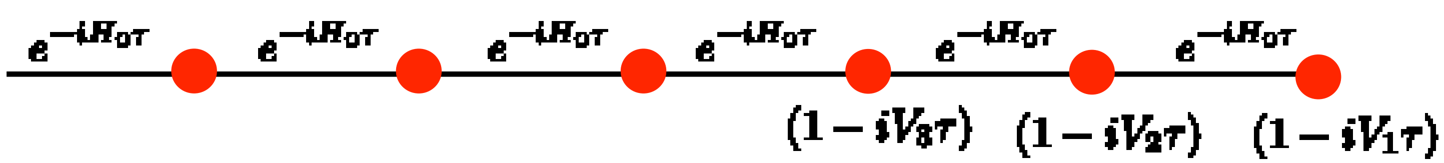
$e^{(H_0+V)} \neq e^{H_0} e^{V}$

Standard trick: discretise the time into small steps and use the fact that $e^{i(H_0+V)\tau} = e^{iH_0\tau} e^{iV\tau} + o(\tau^2)$
i.e., we can split the exponential on each time (the error can be made arbitrarily small):

$$U(t) = e^{-i(H_0+V_N)\tau} e^{-i(H_0+V_{N-1})\tau} e^{-i(H_0+V_{N-2})\tau} \ldots e^{-i(H_0+V_2)\tau} e^{-i(H_0+V_1)\tau}$$

Next we expand the exponentials containing the external field:

$$U(t) = e^{-iH_0\tau}(1 - iV_N\tau) e^{-i(H_0\tau}(1 - iV_{N-1}\tau) e^{-iH_0\tau}(1 - iV_{N-2}\tau) \ldots e^{-iH_0\tau}(1 - iV_2\tau) e^{-iH_0\tau}(1 - iV_1\tau)$$



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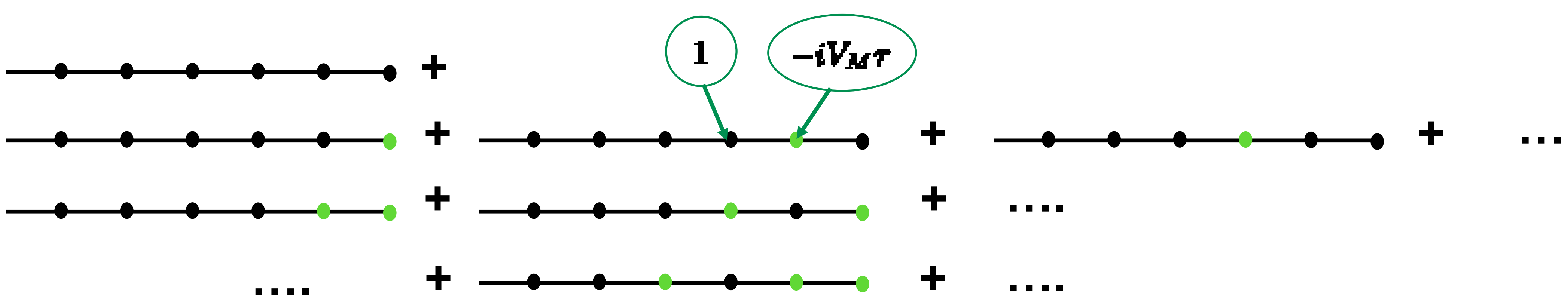
Now we arrange the terms in powers of V:



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$$U(t) = e^{-iH_0 N\tau}$$

$$-i(e^{-iH_0\tau} V_N \tau e^{-iH_0(N-1)\tau} + e^{-iH_0 2\tau} V_{N-1}\tau e^{-iH_0(N-2)\tau} \dots e^{-iH_0(N-1)\tau} V_2 \tau e^{-iH_0\tau} + e^{-iH_0 N\tau} V_1 \tau + \dots)$$

$$= e^{-iH_0 t}\left(1 - i\int_0^t dt' \tilde{V}(t') + (-i)^2 \int_0^t dt' \int_0^{t'} dt'' \tilde{V}(t')\tilde{V}(t'') + \dots\right)$$

$$\equiv e^{-iH_0 t} T \exp\left(-i\int_0^t \tilde{V}(t)\right)$$

Linear response (perturbative) regime

Kubo formula

$H = H_0 + V(t)$

External time-dependent field (el.-mag. field, photon)

[redacted]

Initial state (ground state)

Evolution operator

H0 and V do no
not depend on

T is so called time ordering symbol (sometimes called an time-ordering operator). Note that it is not an operator! The meaning of **T** is the expansion on the line above.
You cannot interpret this expression as “evaluate the integral in the bracket -> exponentiate the result -> apply **T** on the result”!

Standard trick: (
i.e., we can spli

$U(t) = e^{-i(H_0+V}$

Next we expan

$U(t) = e^{-iH_0\tau}(1 \quad iV_N\tau)e^{-i(H_0\tau}(1 - iV_{N-1}\tau)e^{-iH_0\tau}(1 - iV_{N-2}\tau)\ldots e^{-iH_0\tau}(1 - iV_2\tau)e^{-iH_0\tau}(1 - iV_1\tau)$

$U(t) = e^{-iH_0N\tau}$

$-i(e^{-iH_0\tau}V_N\tau e^{-iH_0(N-1)\tau} + e^{-iH_02\tau}V_{N-1}\tau e^{-iH_0(N-2)\tau}\ldots e^{-iH_0(N-1)\tau}V_2\tau e^{-iH_0\tau} + e^{-iH_0N\tau}V_1\tau + \ldots)$

$= e^{-iH_0t}(1 - i\int_0^t dt'\tilde{V}(t') + (-i)^2\int_0^t dt'\int_0^{t'} dt''\tilde{V}(t')\tilde{V}(t'') + \ldots)$ $\qquad \tilde{V}(t) \equiv e^{iH_0t}V(t)e^{-iH_0t}$

$\equiv e^{-iH_0t}T\exp\left(-i\int_0^t \tilde{V}(t)\right)$

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Linear response (perturbative) regime

Kubo formula

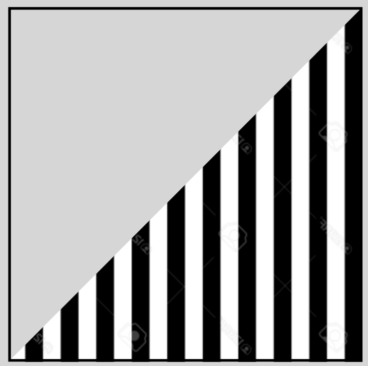
$H = H_0 +$

[redacted]

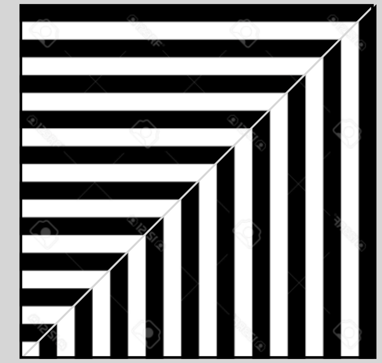
Evolution

H₀ and V d
not depend

$$\int dt' dt''$$



$$= \frac{1}{2} \int dt' dt''$$



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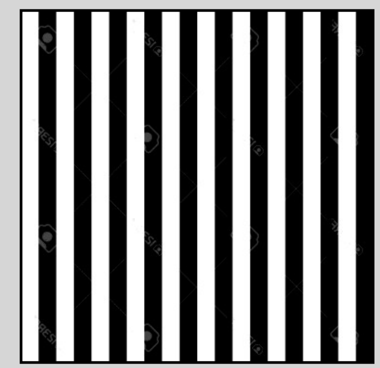

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$$U(t) = e^{-iH \quad N\tau}$$

$$-i(e^{-\quad H_0\tau}V_N\tau e^{-iH_0(N-1)\tau} + e^{-iH_0 2\tau}V_{N-1}\tau e^{-iH_0(N-2)\tau}\ldots e^{-iH_0(N-1)\tau}V_2\tau e^{-iH_0\tau} + e^{-iH_0 N\tau}V_1\tau + \ldots)$$

$$= e^{-iH_0t}(1 - i\int_0^t dt' \tilde{V}(t') + (-i)^2 \int_0^t dt' \int_0^{t'} dt'' \tilde{V}(t')\tilde{V}(t'') + \ldots)$$

$$\tilde{V}(t) \equiv e^{iH_0t}V(t)e^{-iH_0t}$$

$$\equiv e^{-iH_0t} T \exp\left(-i\int_0^t \tilde{V}(t)\right)$$

$$\tilde{V}(t) \equiv e^{iH_0t}V(t)e^{-iH_0t}$$

Linear response (perturbative) regime

Kubo formula

Now we can evaluate the expectation value of operator A in the system evolving with time

$$\langle n(t)|A|n(t)\rangle = \langle n|e^{iHt}Ae^{-iHt}|n\rangle$$
$$\approx \langle n|(1+i\int_0^t dt'\tilde{V}(t'))e^{iH_0t}Ae^{-iH_0t}(1-i\int_0^t dt'\tilde{V}(t'))|n\rangle$$
$$= \langle n|\tilde{A}(t)|n\rangle + i\int_0^t dt'\langle n|[\tilde{V}(t'),\tilde{A}(t)|n\rangle$$

We keep only terms **linear** in V.

$$\langle A(t)\rangle \approx \langle A\rangle_0 + i\int_{-\infty}^t dt'\langle[\tilde{V}(t'),\tilde{A}(t)]\rangle_0$$

In compact form. Note that operators are in so called interaction representation with respect to H_0 (This is indicated by $<>_0$)

We have shifted origin of time integral to infinity, assuming that the perturbation is adiabatically (slowly) turned on (this excludes the transient states that takes place after sudden turning of finite external field)

The formula can be used in thermal equilibrium, in which case $<>_0$ refers to thermal average - trace with $e^{(-H_0/kT)}$.

Linear response (perturbative) regime

Kubo formula

$$\langle A(t)\rangle \approx \langle A\rangle_0 + i\int_{-\infty}^{t} dt' \langle [\tilde{V}(t'), \tilde{A}(t)]\rangle_0$$

A typical external field has the form of a (classical) function (electric field, Zeeman field, vector potential, …) coupled to a typically (semilocal) operator (charge-, spin-, current-density):

$$V(t) = B\phi(t)$$

In the linear response regime the amplitude of the response is linearly proportional to the amplitude of the external field. We want to investigate the trivial temporal (or frequency) relationship.

$$\langle A(t)\rangle_\phi - \langle A\rangle_0 = i\int_{-\infty}^{t} dt' \langle [\tilde{B}(t'), \tilde{A}(t)]\rangle_0 \phi(t') = i\int_{-\infty}^{\infty} dt' \Theta(t-t') \langle [\tilde{B}(t'), \tilde{A}(t)]\rangle_0 \phi(t')$$
$$\equiv \int_{-\infty}^{\infty} dt' \chi_{AB}(t-t')\phi(t')$$

Note, that the expectation value of the commutator depends only on the difference t-t', because H_0 does not depend on time.