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**Condensed matter physics:
from magnetism
to quantum spin liquid I**

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What is condensed matter physics?

- 凝縮系物理、固体物理、物性物理、... in Japanese

From Wikipedia

Condensed matter physics

Article Talk

From Wikipedia, the free encyclopedia

Condensed matter physics is the field of [physics](#) that deals with the macroscopic and microscopic physical properties of [matter](#), especially the [solid](#) and [liquid phases](#), that arise from [electromagnetic forces](#) between [atoms](#) and [electrons](#). More generally, the subject deals with condensed phases of matter: systems of many constituents with strong interactions among them. More exotic condensed phases include the [superconducting](#) phase exhibited by certain materials at extremely low [cryogenic temperatures](#), the [ferromagnetic](#) and [antiferromagnetic](#) phases of [spins](#) on [crystal lattices](#) of atoms, the [Bose–Einstein condensates](#) found in [ultracold atomic systems](#), and [liquid crystals](#). Condensed matter physicists seek to understand the behavior of these phases by experiments to measure various material properties, and by applying the [physical laws of quantum mechanics](#), [electromagnetism](#), [statistical mechanics](#), and other [physics theories](#) to develop mathematical models and predict the properties of extremely large groups of atoms.^[1]

From JPS meeting (日本物理学会)

第79回年次大会（2024年）のキーワード番号

素粒子論領域
素粒子実験領域
理論核物理領域
実験核物理領域
宇宙線・宇宙物理領域
ビーム物理領域 **atom, molecular, optical physics**
領域1 (原子分子、量子エレクトロニクス、放射線)
領域2 (プラズマ)
領域3 (磁性) **magnetism**
領域4 (半導体、メゾスコピック系、量子輸送) **semiconductor**
領域5 (光物性)
領域6 (金属 (液体金属、準結晶)、低温 (超低温、超伝導、密度波))
領域7 (分子性固体) **metal superconductor, density wave**
領域8 (強相関電子系) **strongly correlated electron systems**
領域9 (表面・界面、結晶成長)
領域10 (構造物性 (誘電体、格子欠陥・ナノ構造、X線・粒子線、フォノン))
領域11 (物性基礎論、統計力学、流体物理、応用数学、社会経済物理)
領域12 (ソフトマター物理、化学物理、生物物理) **statistical mechanics**
領域13 (物理教育、物理学史、環境物理)

- Focus on **magnetism** today and tomorrow

Rough outline

Hamiltonian for electrons in atoms

$$\mathcal{H} = - \sum_j^{N_e} \frac{\hbar^2}{2m} \nabla_j^2 - \sum_{\alpha}^{N_i} \frac{\hbar^2}{2M_{\alpha}} \nabla_{\alpha}^2 - \sum_j^{N_e} \sum_{\alpha}^{N_i} \frac{Z_{\alpha} e^2}{|\vec{r}_j - \vec{R}_{\alpha}|} + \sum_{j \ll k}^{N_e} \frac{e^2}{|\vec{r}_j - \vec{r}_k|} + \sum_{\alpha \ll \beta}^{N_j} \frac{Z_{\alpha} Z_{\beta} e^2}{|\vec{R}_{\alpha} - \vec{r}_{\beta}|}$$



Hubbard model

$$\hat{H} = - \sum_{i,j,\sigma} t_{ij} \hat{c}_{i\sigma}^+ \hat{c}_{j\sigma} + \sum_i U_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$



Heisenberg model

$$\hat{H} = \sum_{ij} J_{ij} \hat{S}_i \cdot \hat{S}_j$$



magnetism, quantum spin liquid, ...

Outline

- Brief review of itinerant electron systems
 - Electrons in crystals
 - Second quantization
 - Hubbard models
 - Solving models for simple cases
 - Noninteracting and atomic limits
 - Mean-field approximation
 - Exact diagonalization (2 sites)
 - Strong coupling limit: Heisenberg model (spin system)
- Magnetism and quantum spin liquid
 - Spin models
 - Frustrated magnetism and quantum spin liquid
 - Kitaev honeycomb spin liquid

Rough outline

Hamiltonian for electrons in atoms

$$\mathcal{H} = - \sum_j^{N_e} \frac{\hbar^2}{2m} \nabla_j^2 - \sum_{\alpha}^{N_i} \frac{\hbar^2}{2M_{\alpha}} \nabla_{\alpha}^2 - \sum_j^{N_e} \sum_{\alpha}^{N_i} \frac{Z_{\alpha} e^2}{|\vec{r}_j - \vec{R}_{\alpha}|} + \sum_{j \ll k}^{N_e} \frac{e^2}{|\vec{r}_j - \vec{r}_k|} + \sum_{\alpha \ll \beta}^{N_j} \frac{Z_{\alpha} Z_{\beta} e^2}{|\vec{R}_{\alpha} - \vec{r}_{\beta}|}$$

Second quantization

Hubbard model

$$\hat{H} = - \sum_{i,j,\sigma} t_{ij} \hat{c}_{i\sigma}^+ \hat{c}_{j\sigma} + \sum_i U_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

Heisenberg model

$$\hat{H} = \sum_{ij} J_{ij} \hat{S}_i \cdot \hat{S}_j$$

magnetism, quantum spin liquid, ...

For simplicity, consider 2 free electrons

$$H = -\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial r_1^2} + \frac{\partial^2}{\partial r_2^2} \right)$$

$$H \Psi(r_1, r_2) = E \Psi(r_1, r_2)$$

Solve the eigenvalue problem and **antisymmetrize** the wave function for fermion

$$\Psi(r_1, r_2) = \frac{1}{\sqrt{2}} (\varphi_\alpha(r_1) \varphi_\beta(r_2) - \varphi_\beta(r_1) \varphi_\alpha(r_2))$$

$\varphi_a(r)$ is defined as

$$\text{for } h_f = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial r_f^2}$$

$$h_f \varphi_\alpha(r_f) = E_\alpha \varphi_\alpha(r_f)$$

Motivation: Simplify the notation

- 2-site case is simple
- For $N > 2$ sites, Ψ is Slater determinant
- We would like to simplify the notation of the state
 - Omit **coordinates** (r_1, r_2, \dots)
 - Omit **permutations**
(Antisymmetrization for fermions)
- Introduce
 - Dirac state $|n_\alpha\rangle$
(number of electron 0 or 1 for orbital α)
 - Creation and annihilation operators for fermions

Remove coordinate

$$\varphi_{\alpha\beta}(r_1, r_2) = \frac{1}{\sqrt{2}} (\varphi_\alpha(r_1) \varphi_\beta(r_2) - \varphi_\beta(r_1) \varphi_\alpha(r_2))$$
$$= \frac{1}{\sqrt{2}} (\langle r_1 | n_\alpha \rangle \langle r_2 | n_\beta \rangle - \langle r_1 | n_\beta \rangle \langle r_2 | n_\alpha \rangle)$$

of electrons (0 or 1)
for orbital α

$$= \langle r_1 r_2 | \frac{1}{\sqrt{2}} (| n_\alpha n_\beta \rangle - | n_\beta n_\alpha \rangle) \rangle$$

$$=: \underbrace{\langle r_1 r_2 | \varphi \rangle}_{\text{coordinates are separated}}$$

In general,

$$|\varphi\rangle = \sum_{n_1, n_2} \frac{f(n_1, n_2)}{\text{coefficient}} |n_1 n_2\rangle$$

Permutation \rightarrow Commutator

Rewrite single electron states by the creation operator

$$|n_\alpha\rangle = \hat{c}_\alpha^+ |0\rangle$$

$|0\rangle$ is defined as

$$\begin{cases} \hat{c}_\alpha |0\rangle = 0 & \leftarrow \text{cannot remove} \\ & \text{electron from vacuum} \\ \langle 0|0\rangle = 1 & \leftarrow \text{normalization} \end{cases}$$

Assume anti commutation relation

$$\hat{c}_\alpha^+ \hat{c}_\beta^+ = - \hat{c}_\beta^+ \hat{c}_\alpha^+$$

Now, the order of electrons (permutations)
is encoded in the order of operator

$$\langle n_\alpha n_\beta \rangle = \hat{c}_\beta^+ \hat{c}_\alpha^+ |0\rangle = - \hat{c}_\alpha^+ \hat{c}_\beta^+ |0\rangle = - \langle n_\beta n_\alpha \rangle$$

Construct operator \hat{H} from H

$$H \Psi(r_1, r_2) = E \Psi(r_1, r_2)$$

$$\hat{H} |\psi\rangle = E |\psi\rangle$$

with

$$\begin{cases} |\psi\rangle = \sum_{n_1, n_2} f(n_1, n_2) |n_1, n_2\rangle \\ |n_\alpha\rangle = \hat{c}_\alpha^\dagger |0\rangle \end{cases}$$

Construct \hat{H} from H : second quantization

But how?

Preparation: Introduce field operator

Expand $|r\rangle$ by $|n_\alpha\rangle$

$\xrightarrow{\text{State at position } r}$ $\xrightarrow{\text{single electron in state } \alpha}$

Using $1 = \sum_\alpha |n_\alpha\rangle \langle n_\alpha|$,

$$|r\rangle = \sum_\alpha |n_\alpha\rangle \langle n_\alpha| r \rangle = \sum_\alpha (r | n_\alpha \rangle)^* |n_\alpha \rangle = \sum_\alpha \varphi_\alpha^*(r) |n_\alpha \rangle$$

$$= \sum_\alpha \underbrace{\varphi_\alpha^*(r)}_{!!} \underbrace{\hat{C}_\alpha^\dagger |0\rangle}_{!!}$$

$\hat{\Psi}^\dagger(r)$: field operator

Note that $\varphi_\alpha(r)$ is orthonormalized and complete:

$$\begin{cases} \int dr \varphi_\alpha^*(r) \varphi_\beta(r) = \delta_{\alpha\beta} \\ \sum \varphi_\alpha(r) \varphi_\alpha(r') = \delta(r-r') \end{cases}$$

Conversely,

$$|n_\alpha\rangle = \underbrace{\int dr |r\rangle \langle r| n_\alpha}_{\parallel} = \underbrace{\int dr \varphi_\alpha(r) |r\rangle}_{\text{mm}} = \int dr \varphi_\alpha(r) \underbrace{\hat{\Psi}^\dagger(r) |0\rangle}_{\text{mmmm}}$$

$$\hat{C}_\alpha^\dagger |0\rangle$$

$$\therefore \hat{C}_\alpha^\dagger = \int dr \varphi_\alpha(r) \hat{\Psi}^\dagger(r)$$

Second quantized Hamiltonian

Field operator :

$$\hat{\Psi}^+(r) := \sum_{\alpha} \varphi_{\alpha}^*(r) \hat{c}_{\alpha}^+$$

\hat{H} can be constructed from H and $\hat{\Psi}^+(r)$:
(for free fermions)

$$\hat{H} = \int dr \quad \hat{\Psi}^+(r) \quad H \quad \hat{\Psi}(r)$$

Check by taking an example

Example single electron case : $H\psi_\alpha(r) = E_\alpha \psi_\alpha(r)$

$$\begin{aligned} \hat{H} &= \int dr \hat{\Psi}^f(r) H \hat{\Psi}(r) && \xrightarrow{\text{use } \hat{\Psi}(r) = \sum \psi_\alpha^*(r) \hat{C}_\alpha^\dagger} \sum \psi_\alpha^*(r) \hat{C}_\alpha^\dagger \\ &= \int dr \sum_\alpha \psi_\alpha^*(r) \hat{C}_\alpha^\dagger H \sum_\beta \psi_\beta(r) \hat{C}_\beta \\ &= \sum_{\alpha\beta} \left(\int dr \underbrace{\psi_\alpha^*(r) H \psi_\beta(r)}_{\text{H}} \right) \hat{C}_\alpha^\dagger \hat{C}_\beta \\ &= \sum_{\alpha\beta} \left(\int dr \underbrace{\psi_\alpha^*(r) E_\beta \psi_\beta(r)}_{\text{H}} \right) \hat{C}_\alpha^\dagger \hat{C}_\beta \\ &= \sum_{\alpha\beta} E_\beta \underbrace{\int dr \psi_\alpha^*(r) \psi_\beta(r)}_{\frac{\delta}{\delta \alpha\beta}} \hat{C}_\alpha^\dagger \hat{C}_\beta \\ &= \sum_\alpha E_\alpha \hat{C}_\alpha^\dagger \hat{C}_\alpha \end{aligned}$$

Then,

$$\begin{aligned} \hat{H}(n_\beta) &= \sum_\alpha E_\alpha \underbrace{\hat{C}_\alpha^\dagger \hat{C}_\alpha}_{\hat{C}_\beta^\dagger \hat{C}_\beta(0)} \hat{C}_\beta^\dagger(0) = E_\beta \hat{C}_\beta^\dagger(0) = E_\beta |n_\beta\rangle \\ &= \delta_{\alpha\beta} - \hat{C}_\beta^\dagger \hat{C}_\alpha \end{aligned}$$

Second quantize 2-body interaction

When we have , for example,

$$V(r_1, r_2) = \frac{1}{|r_1 - r_2|}, \quad \begin{matrix} \text{2-body} \\ \text{term} \end{matrix}$$

second quantized Hamiltonian is

$$\begin{aligned}\hat{V} &= \frac{1}{2} \int dr \int dr' \hat{\Psi}^+(r) \hat{\Psi}^+(r') V(r, r') \hat{\Psi}(r') \hat{\Psi}(r) \\ &= : \sum_{\alpha\beta\gamma\delta} V_{\alpha\beta\gamma\delta} \hat{C}_\alpha^+ \hat{C}_\beta^+ \hat{C}_\gamma \hat{C}_\delta\end{aligned}$$

Hamiltonian in crystals

In periodic potential, Hamiltonian is

$$H(r) = \sum_i H_i (r - R_i)$$

atom index Hamiltonian
of atoms
at site R_i

$\begin{matrix} 0 & 0 & 0 & 0 & 0 & 0 \\ i=1 & i=2 & i=3 & \dots \end{matrix}$

We should take into account

atom site i and spin degrees of freedom σ
(\uparrow, \downarrow)

Field operator:

$$\hat{\Psi}_{i\sigma}^+(r) = \sum_{i\sigma} \varphi_{i\sigma}^*(r) \hat{c}_{i\sigma}^+ |0\rangle$$

atom index spin

Up to 2-body terms:

$$\hat{H} = - \sum_{if\sigma} t_{if\sigma} \hat{c}_{i\sigma}^+ \hat{c}_{f\sigma} + \sum_{ijhl} V_{ijkl} \hat{c}_{i\sigma}^+ \hat{c}_{j\sigma}^+ \hat{c}_{h\sigma} \hat{c}_{l\sigma}$$

$\sigma\sigma'$

add \ominus because of $-\frac{\hbar^2}{2m} \nabla^2$

Further simplification → Hubbard model

- To further simplify the model, consider

- Nearest neighbor i, j for t_{ij}

$$\rightarrow t_{ij} = :t \text{ for } |i-j|=1$$

- Onsite i, j, k, l for V_{ijkl}

$$\hat{H} = - \sum_{i,j,\sigma} t_{ij\sigma} \hat{c}_{i\sigma}^+ \hat{c}_{j\sigma} + \sum_{ijkl} V_{ijkl} \hat{c}_{i\sigma}^+ \hat{c}_{j\sigma}^+ \hat{c}_{k\sigma} \hat{c}_{l\sigma}$$
$$\rightarrow V_{iiii} = :U$$

- We finally obtain the Hubbard model

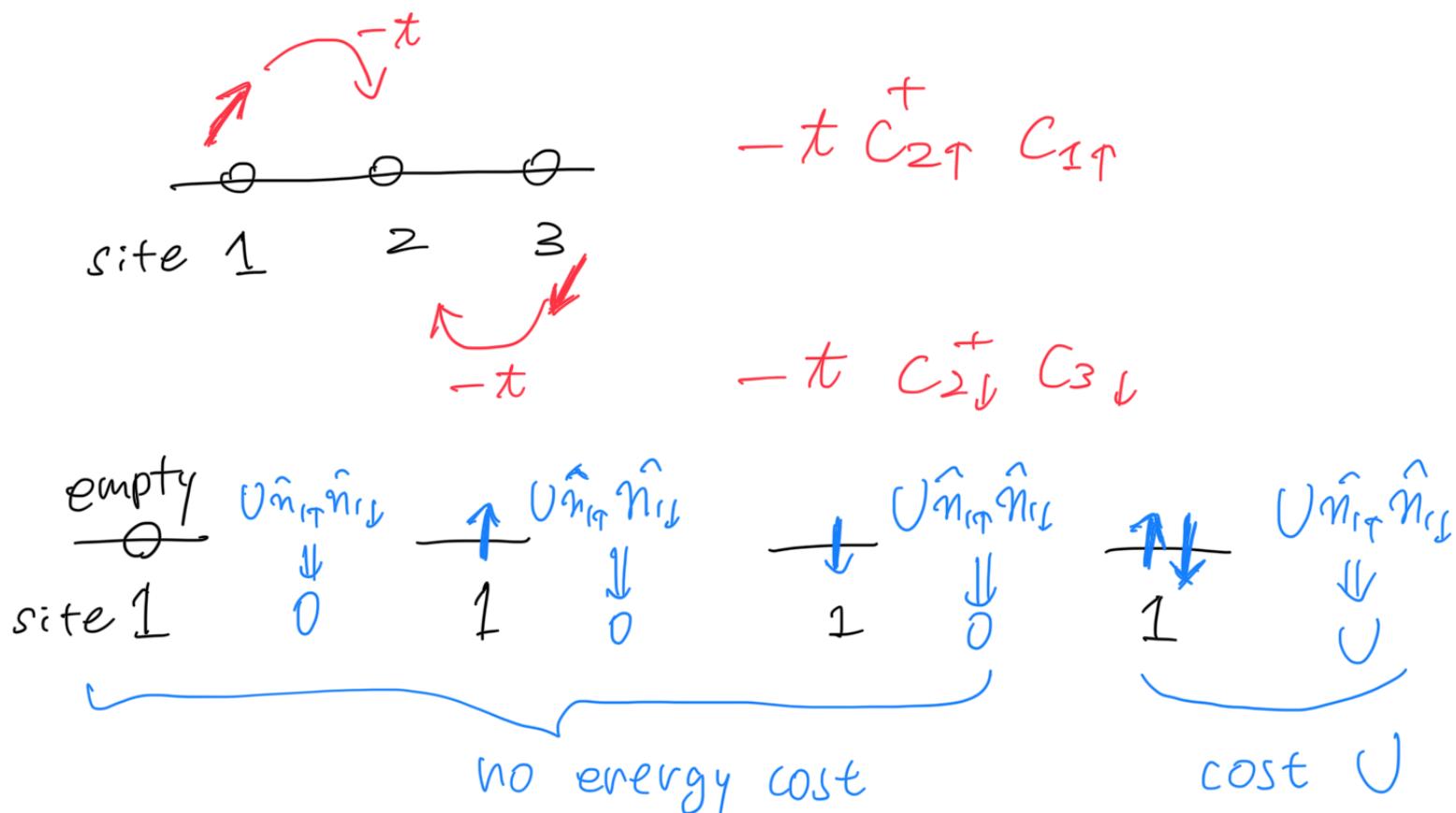
$$\hat{H} = -t \sum_{\langle i,j \rangle} (\hat{c}_{i\sigma}^+ \hat{c}_{j\sigma} + \hat{c}_{j\sigma}^+ \hat{c}_{i\sigma})$$

$\langle \cdot \rangle$ denotes nearest neighbors

$$+ U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

Hubbard model

$$\hat{H} = - \sum_{i,j,\sigma} t_{ij} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \sum_i U_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$



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Hubbard model

$$\hat{H} = - \sum_{i,j,\sigma} t_{ij} \hat{c}_{i\sigma}^+ \hat{c}_{j\sigma} + \sum_i U_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$



Heisenberg model

$$\hat{H} = \sum_{ij} J_{ij} \hat{S}_i \cdot \hat{S}_j$$



magnetism, quantum spin liquid, ...

Several limits / Solve by approximation

- $U=0$ limit (noninteracting limit)
 - Tight-bonding model, free fermion system
- $t=0$ limit
 - Atomic limit
- Mean-field approximation
 - Antiferromagnetic order for bipartite lattices
- 2-site model
 - Relation to the spin model (Heisenberg model)

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Noninteracting limit ($U=0$)

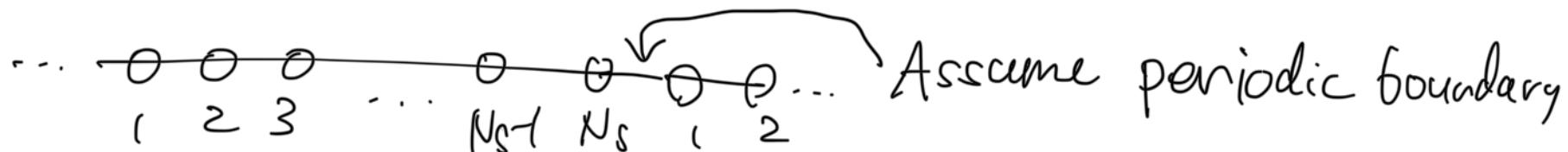
$$\hat{H} = -t \sum_{\langle i,j \rangle} (\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \hat{c}_{j\sigma}^\dagger \hat{c}_{i\sigma})$$

Can be solved by Fourier transformation

$$\hat{c}_{i\sigma} = \frac{1}{\sqrt{N_s}} \sum_{\vec{k}} e^{i\vec{k} \cdot \vec{r}_i} \hat{c}_{\vec{k}\sigma} \quad (N_s : \# \text{ of sites})$$

For example, in 1D chain,

$$\hat{H} = -t \sum_i (\hat{c}_{i\sigma}^\dagger \hat{c}_{i+1\sigma} + \hat{c}_{i+\sigma}^\dagger \hat{c}_{i\sigma})$$



Noninteracting limit ($U=0$)

Using the fact that

$$\begin{aligned} & \sum_i \hat{c}_{i\sigma}^\dagger \hat{c}_{i+\ell\sigma} \\ &= \sum_i \frac{1}{\sqrt{N_s}} \sum_k e^{-ikr_i} \hat{c}_{k\sigma} + \frac{1}{\sqrt{N_s}} \sum_k e^{i\ell(k+r_i)} \hat{c}_{k\sigma} \\ &= \underbrace{\sum_{\ell k} \frac{1}{N_s} \sum_i e^{-i(\ell-k)r_i}}_{=\delta_{\ell k}} \cdot e^{i\ell k} \hat{c}_{k\sigma}^\dagger \hat{c}_{k\sigma} \\ &= \sum_k e^{i\ell k} \hat{c}_{k\sigma}^\dagger \hat{c}_{k\sigma}, \end{aligned}$$

we obtain

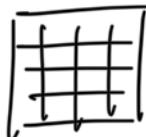
$$\hat{H} = -t \sum_k (e^{ik} + e^{-ik}) \hat{c}_{k\sigma}^\dagger \hat{c}_{k\sigma} = \sum_k \epsilon_k \hat{c}_k^\dagger \hat{c}_k$$

with $\epsilon_k := -2t \cos k$

Noninteracting limit ($U=0$)

1D 

$$\epsilon_k = -2t \cos k$$

2D 

$$\epsilon_k = -2t (\cos k_x + \cos k_y)$$

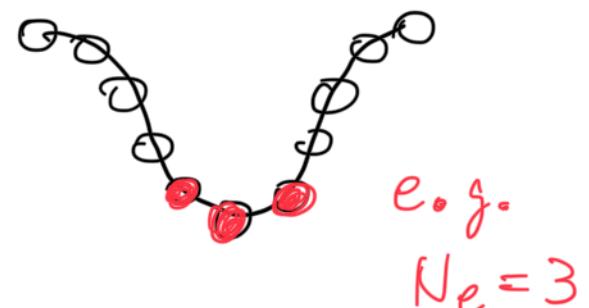
3D 

$$\epsilon_k = -2t (\cos k_x + \cos k_y + \cos k_z)$$

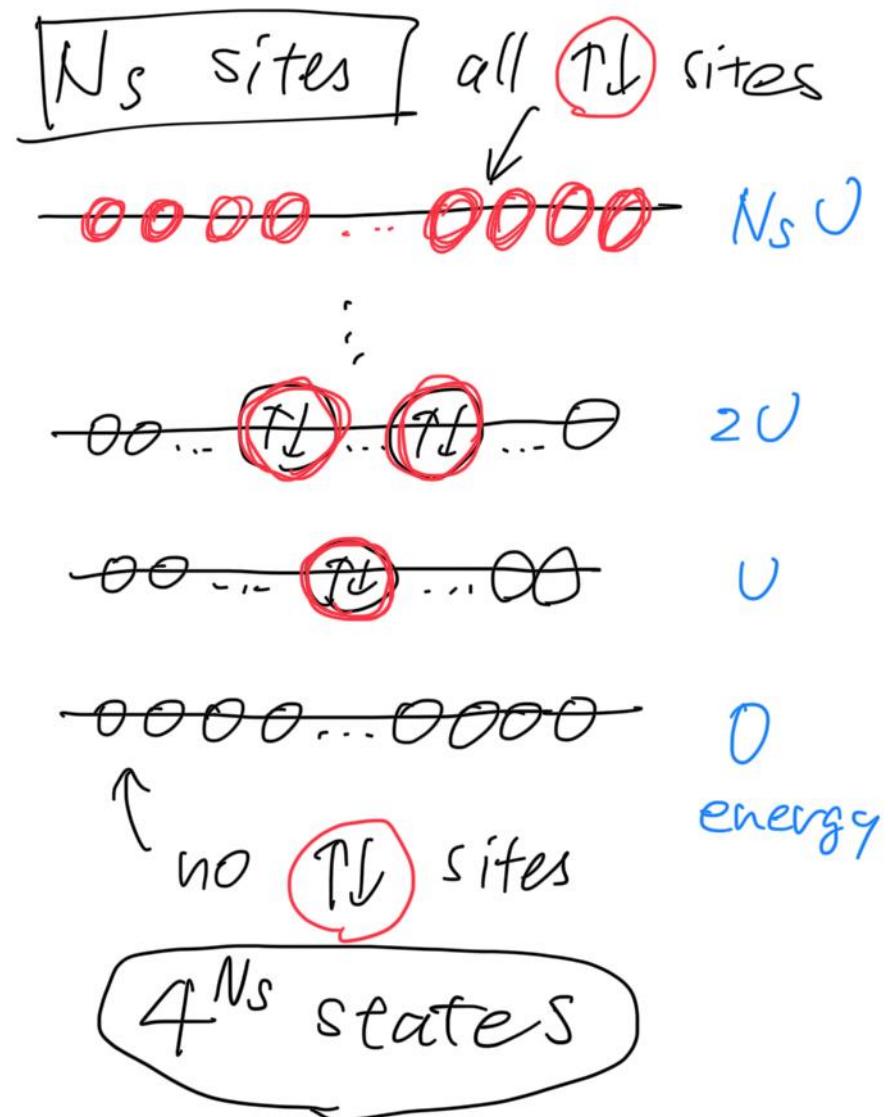
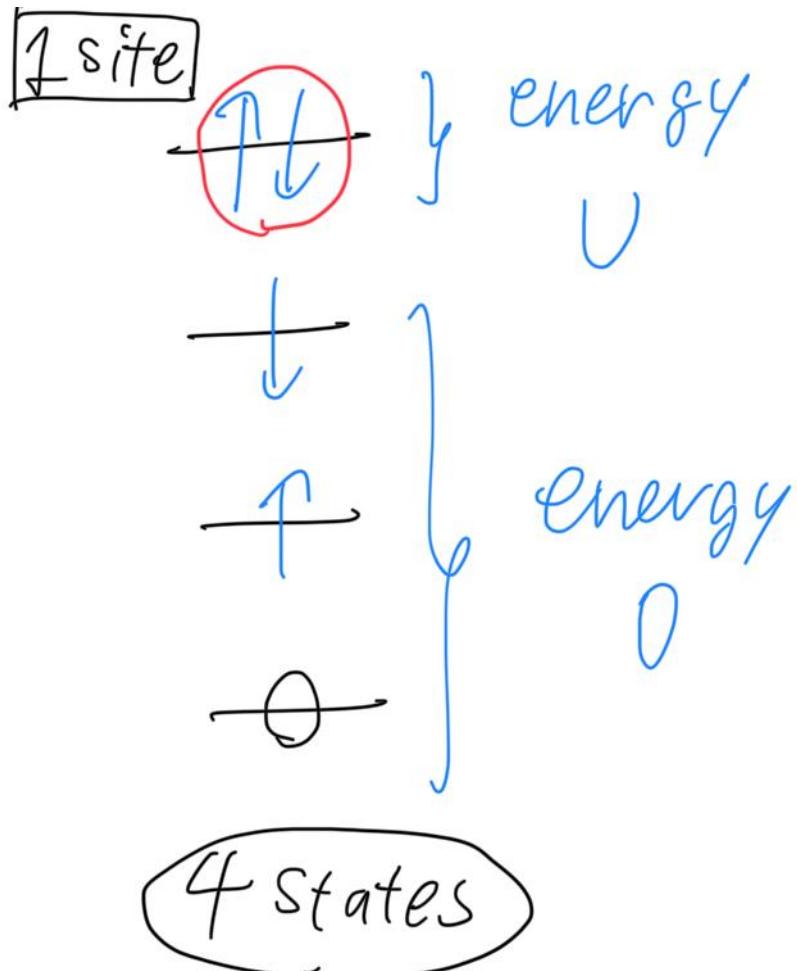
⋮

Ground state energy :

$$E_{GS} = \sum_{\substack{k: \text{lowest} \\ N_e \text{ states}}} \epsilon_k$$



Atomic limit ($t=0$)



Several limits / Solve by approximation

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Mean-field (MF) approximation

$$\hat{A}\hat{B}$$

$$= [\langle \hat{A} \rangle + (\hat{A} - \langle \hat{A} \rangle)][\langle \hat{B} \rangle + (\hat{B} - \langle \hat{B} \rangle)]$$

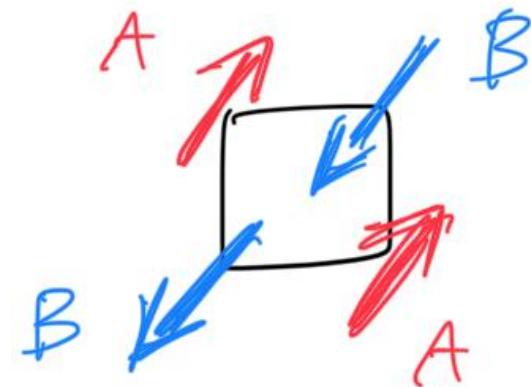
$$\begin{aligned} &= \langle \hat{A} \rangle \langle \hat{B} \rangle + \langle \hat{A} \rangle (\hat{B} - \langle \hat{B} \rangle) + (\hat{A} - \langle \hat{A} \rangle) \langle \hat{B} \rangle \\ &\quad + (\hat{A} - \langle \hat{A} \rangle) (\hat{B} - \langle \hat{B} \rangle) \quad \text{Throw away fluctuations!} \end{aligned}$$

$$\sim \langle \hat{A} \rangle \langle \hat{B} \rangle + \langle \hat{A} \rangle (\hat{B} - \langle \hat{B} \rangle) + (\hat{A} - \langle \hat{A} \rangle) \langle \hat{B} \rangle$$

$$= \langle \hat{A} \rangle \hat{B} + \hat{A} \langle \hat{B} \rangle - \langle \hat{A} \rangle \langle \hat{B} \rangle$$

Mean-field (MF) approximation

- Focus on the case
- Number of sites $N_s = \text{Number of electrons } N_e$
- Often called “half filling” (because $N_\uparrow = N_\downarrow = N_s/2$)
- For hypercubic lattices (chain, square, cube, ...), the ground state can be calculated (numerically exactly), and it shows
 - long-range antiferromagnetic order for 2D, 3D, 4D, ...
 - quasi-long-range antiferromagnetic order for 1D
- Apply MF approx. to check antiferromagnetism



Mean-field (MF) approximation

$$\hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \sim \langle \hat{n}_{i\uparrow} \rangle \hat{n}_{i\downarrow} + \hat{n}_{i\uparrow} \langle \hat{n}_{i\downarrow} \rangle - \langle \hat{n}_{i\uparrow} \rangle \langle \hat{n}_{i\downarrow} \rangle$$

$$H = -t \sum_{i,r} \left(\hat{c}_{i\sigma}^+ \hat{c}_{i+r\sigma} + \hat{c}_{i+r\sigma}^+ \hat{c}_{i\sigma} \right) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

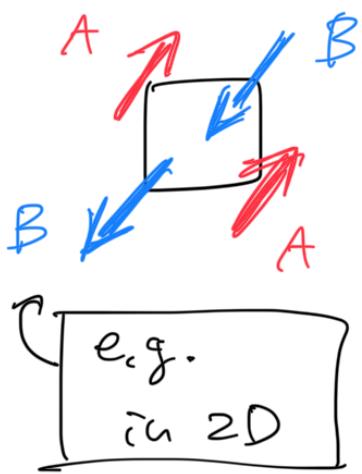
$$\sim \sum_k \varepsilon_k \hat{c}_{k\uparrow}^+ \hat{c}_{k\downarrow} \quad \text{Fourier transform}$$

MF approx.

$$+ U \sum_i \left[\langle \hat{n}_{i\uparrow} \rangle \hat{n}_{i\downarrow} + \hat{n}_{i\uparrow} \langle \hat{n}_{i\downarrow} \rangle - \langle \hat{n}_{i\uparrow} \rangle \langle \hat{n}_{i\downarrow} \rangle \right]$$

Mean-field (MF) approximation

Assume staggered antiferromagnet



$$\langle m_{A\uparrow} \rangle = \frac{1}{2} + m \quad \langle m_{B\uparrow} \rangle = \frac{1}{2} - m$$

$$\langle m_{A\downarrow} \rangle = \frac{1}{2} - m \quad \langle m_{B\downarrow} \rangle = \frac{1}{2} + m$$

$$\langle m_{A\uparrow} + m_{A\downarrow} \rangle = \langle m_{B\uparrow} + m_{B\downarrow} \rangle = 1$$

$$\langle S_A^z \rangle = \frac{1}{2} (\langle m_{A\uparrow} \rangle - \langle m_{A\downarrow} \rangle) = m \in [0, \frac{1}{2}]$$

$$\langle S_B^z \rangle = \frac{1}{2} (\langle m_{B\uparrow} \rangle - \langle m_{B\downarrow} \rangle) = -m$$

For site $i = A$ or B ,

$$\langle m_{i\uparrow} \rangle = \frac{1}{2} + m (-1)^{r_i} = \frac{1}{2} + m e^{i Q r_i}$$

$$\langle m_{i\downarrow} \rangle = \frac{1}{2} - m (-1)^{r_i} = \frac{1}{2} - m e^{i Q r_i}$$

($\theta = \pi$ in 2D, $Q = (\pi, \pi)$ in 2D, $Q = (\pi, \pi, \pi)$ in 3D)

Mean-field (MF) approximation

Using

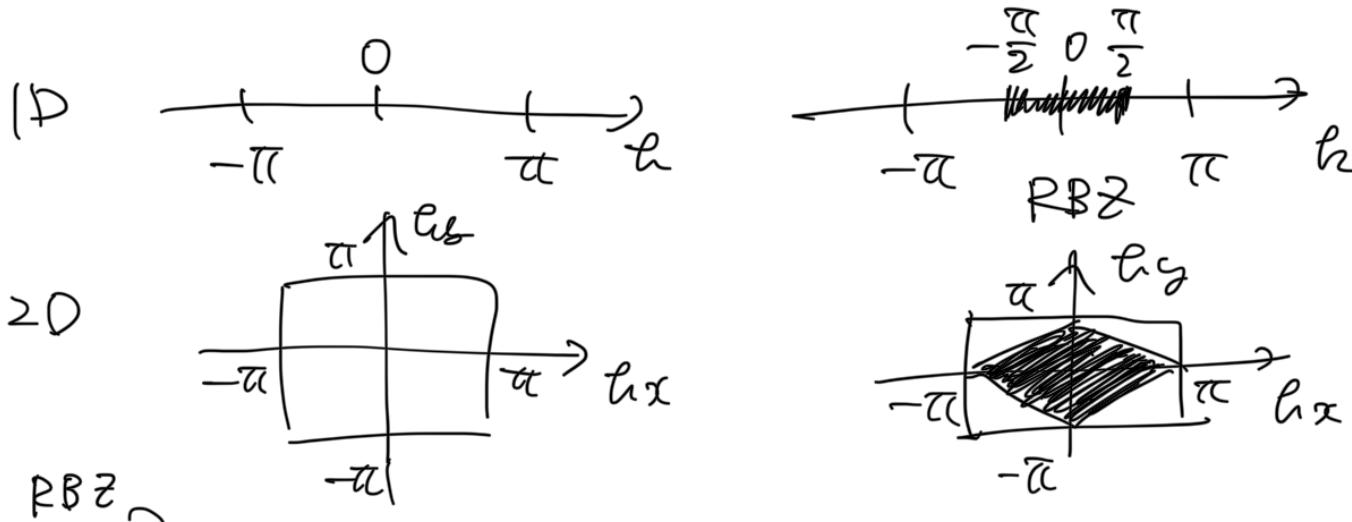
$$\begin{aligned}\sum_i \langle n_{i\uparrow} \rangle n_{i\downarrow} &= \sum_i \left(\frac{1}{2} + m e^{i\Omega V_i} \right) c_{i\uparrow}^\dagger c_{i\downarrow} \\ &= \frac{1}{2} \sum_a c_{a\uparrow}^\dagger c_{a\downarrow} + m \sum_a c_{a\uparrow}^\dagger c_{a-\alpha\downarrow} \text{ etc}\end{aligned}$$

We have

$$\begin{aligned}H &\sim \sum_{a\sigma} \epsilon_{a\sigma} c_{a\sigma}^\dagger c_{a\sigma} + \frac{\Omega}{2} \sum_{a\sigma} c_{a\sigma}^\dagger c_{a\sigma} \\ &+ jm \sum_a (c_{a\uparrow}^\dagger c_{a-\alpha\downarrow} - c_{a\downarrow}^\dagger c_{a-\alpha\uparrow})\end{aligned}$$

Mean-field (MF) approximation

Rewrite sum by reduced Brillouin zone (RBZ)



$$\begin{aligned}
 H \sim & \sum_{\sigma} \left(E_{h\sigma} C_{h\sigma} + E_{h\bar{\sigma}} C_{h\bar{\sigma}}^\dagger + C_{h\sigma}^\dagger C_{h\bar{\sigma}} \right) \\
 & + \frac{U}{2} \sum_{\sigma} \left(C_{h\sigma}^\dagger C_{h\sigma} + C_{h\bar{\sigma}}^\dagger C_{h\bar{\sigma}} \right) \\
 & + U_m \sum_h \left(C_{h\downarrow}^\dagger C_{h\bar{\sigma}\downarrow} + C_{h\bar{\sigma}\downarrow}^\dagger C_{h\downarrow} \right. \\
 & \quad \left. - C_{h\uparrow}^\dagger C_{h\bar{\sigma}\uparrow} - C_{h\bar{\sigma}\uparrow}^\dagger C_{h\uparrow} \right)
 \end{aligned}$$

Mean-field (MF) approximation

$$H \sim \sum_{\sigma} \left(C_{\sigma\sigma}^+ C_{h-\bar{Q}\sigma}^- \right)$$
$$\begin{pmatrix} E_h + \frac{U}{2} & -\sigma U m \\ -\sigma U m & E_{h-\bar{Q}} + \frac{U}{2} \end{pmatrix} \begin{pmatrix} C_{\sigma\sigma} \\ C_{h-\bar{Q}\sigma} \end{pmatrix}$$
$$\sigma = \begin{cases} + & \text{for } \uparrow \\ - & \text{for } \downarrow \end{cases}$$

After diagonalizing the 2×2 matrix, we have

$$H = \sum_{\sigma} \tilde{E}_h \mathcal{D}_{\sigma\sigma}^+ \mathcal{D}_{\sigma\sigma}$$

with $\tilde{E}_h = \frac{U}{2} \pm \sqrt{\epsilon_h^2 + U^2 m^2}$

Mean-field (MF) approximation

Magnetization can be obtained from
self-consistent equation

$$\left(\frac{1}{2}\right)^n = \frac{1}{N_s} \sum_{\sigma} \langle n_{i\sigma} \rangle = \frac{1}{N_s} \sum_{\sigma} \langle c_{i\sigma}^\dagger c_{i\sigma} \rangle$$

For $N_s \rightarrow \infty$ limit (D : spatial dimension)

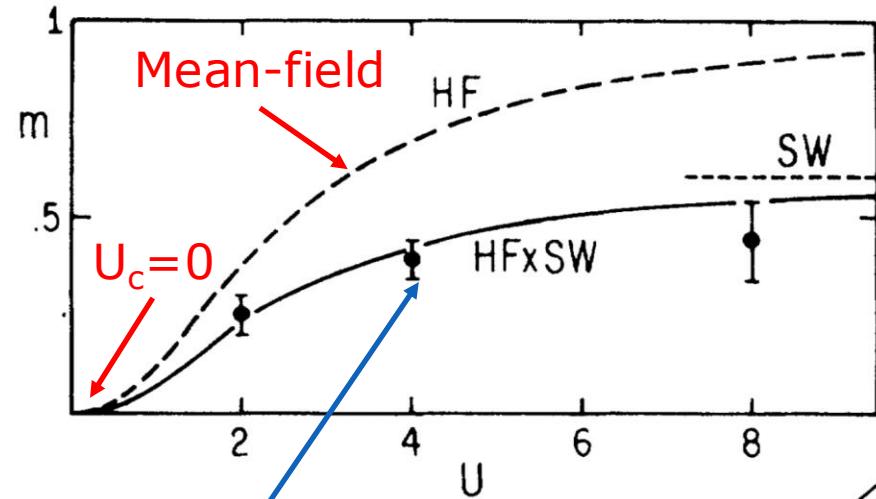
$$T = U \int \frac{d^D k}{(2\pi)^D} \frac{1}{\sqrt{\varepsilon_w^2 + U^2 m^2}}$$

$$= U \int_{\varepsilon_{\min}}^{\varepsilon_{\max}} d\varepsilon \frac{\rho(\varepsilon)}{\sqrt{\varepsilon^2 + U^2 m^2}}$$

Density of states in hypercubic systems

Transition occurs at $U_c = 0$

$$\langle c_m \rangle \sim \begin{cases} \frac{t}{U} e^{-2\pi t/U} & (D=1, 3) \\ \frac{t}{U} e^{-2\pi \sqrt{t}/U} & (D=2) \end{cases}$$



Numerically exact
(quantum Monte Carlo)

J. E. Hirsch, PRB.31.4403('85)

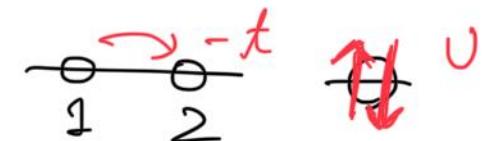
J. E. Hirsch and S. Tang, PRL.62.591('88)

Several limits / Solve by approximation

- $U=0$ limit (noninteracting limit)
 - Tight-bonding model, free fermion system
- $t=0$ limit
 - Atomic limit
- Mean-field approximation
 - Antiferromagnetic order for bipartite lattices
- 2-site model
 - Relation to the spin model (Heisenberg model)

2-site Hubbard model

$$H = -t \sum_{\sigma} (C_{1\sigma}^+ C_{2\sigma} + C_{2\sigma}^+ C_{1\sigma})$$



$$+ U \left[(n_{1\uparrow} - \frac{1}{2})(n_{1\downarrow} - \frac{1}{2}) + (n_{2\uparrow} - \frac{1}{2})(n_{2\downarrow} - \frac{1}{2}) \right]$$

at half filling

$$|\text{basis}\rangle = \begin{pmatrix} |\uparrow\rangle \\ |\uparrow\uparrow\rangle \\ |\uparrow\downarrow\rangle \\ |\uparrow\downarrow\downarrow\rangle \end{pmatrix} \otimes \begin{pmatrix} |\uparrow\rangle \\ |\uparrow\uparrow\rangle \\ |\uparrow\downarrow\rangle \\ |\uparrow\downarrow\downarrow\rangle \end{pmatrix} \quad 16 \text{ states}$$

In principle, one can solve the model

by diagonalizing a 16×16 matrix.

→ Let's cut corners.

2-site Hubbard model

Total spin and total S^z are conserved

$$[H, S_{\text{tot}}^2] = [H, S_{\text{tot}}^z] = 0$$

$$\left(\begin{array}{l} S_{\text{tot}}^2 = S_1^2 + S_2^2, \quad S_i^2 = (S_i^x)^2 + (S_i^y)^2 + (S_i^z)^2 \\ S_{\text{tot}}^z = S_1^z + S_2^z, \quad S_i^z = \frac{1}{2}(c_{i\uparrow}^+ c_{i\uparrow} - c_{i\downarrow}^+ c_{i\downarrow}) \\ S_i^x = \frac{1}{2}(c_{i\uparrow}^+ c_{i\downarrow} + c_{i\downarrow}^+ c_{i\uparrow}), \quad S_i^y = \frac{1}{2i}(c_{i\uparrow}^+ c_{i\downarrow} - c_{i\downarrow}^+ c_{i\uparrow}) \end{array} \right)$$

Use eigenstates of S_{tot}^2 and S_{tot}^z
to describe eigenstates of Hamiltonian H

2-site Hubbard model

Eigenstates of S_{tot}^2 , S_{tot}^z at half filling

	S_{tot}^2	S_{tot}^z
$ \phi_{S1}\rangle = \frac{1}{\sqrt{2}}(\uparrow,\downarrow\rangle - \downarrow,\uparrow\rangle)$	0	0
$ \phi_{S2}\rangle = \uparrow\downarrow, 0\rangle$	0	0
$ \phi_{S3}\rangle = 0, \uparrow\downarrow\rangle$	0	0
$ \phi_{\pm 1}\rangle = \uparrow, \uparrow\rangle$	1	+1
$ \phi_{\pm 2}\rangle = \frac{1}{\sqrt{2}}(\uparrow,\downarrow\rangle + \downarrow,\uparrow\rangle)$	1	0
$ \phi_{\pm 3}\rangle = \downarrow,\downarrow\rangle$	1	-1

2-site Hubbard model

$$\Psi = (|\phi_{s_1}\rangle |\phi_{s_2}\rangle |\phi_{s_3}\rangle |\phi_{t_1}\rangle |\phi_{t_2}\rangle |\phi_{t_3}\rangle)$$

$$H = \Psi^\dagger M \Psi$$

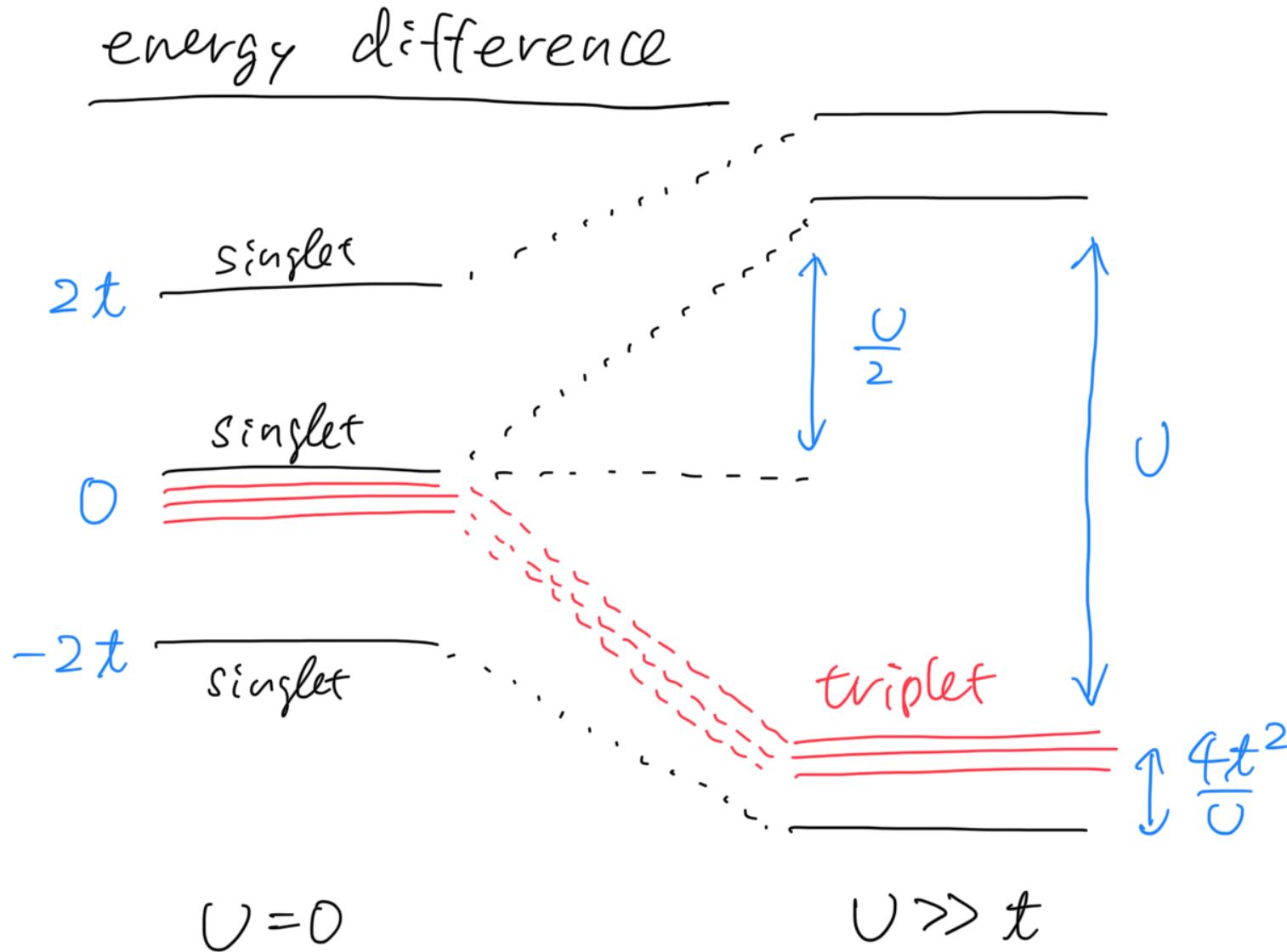
3x3 matrix for singlet states

$$M = \begin{pmatrix} \begin{matrix} -\frac{U}{2} & -\sqrt{2}t & -\sqrt{2}t \\ -\sqrt{2}t & \frac{U}{2} & 0 \\ -\sqrt{2}t & 0 & \frac{U}{2} \end{matrix} & \begin{matrix} 0 \\ 0 \\ 0 \end{matrix} \\ \begin{matrix} 0 \\ 0 \\ 0 \end{matrix} & \begin{matrix} -\frac{U}{2} & 0 & 0 \\ 0 & -\frac{U}{2} & 0 \\ 0 & 0 & -\frac{U}{2} \end{matrix} \end{pmatrix}$$

block diagonalized for triplet states

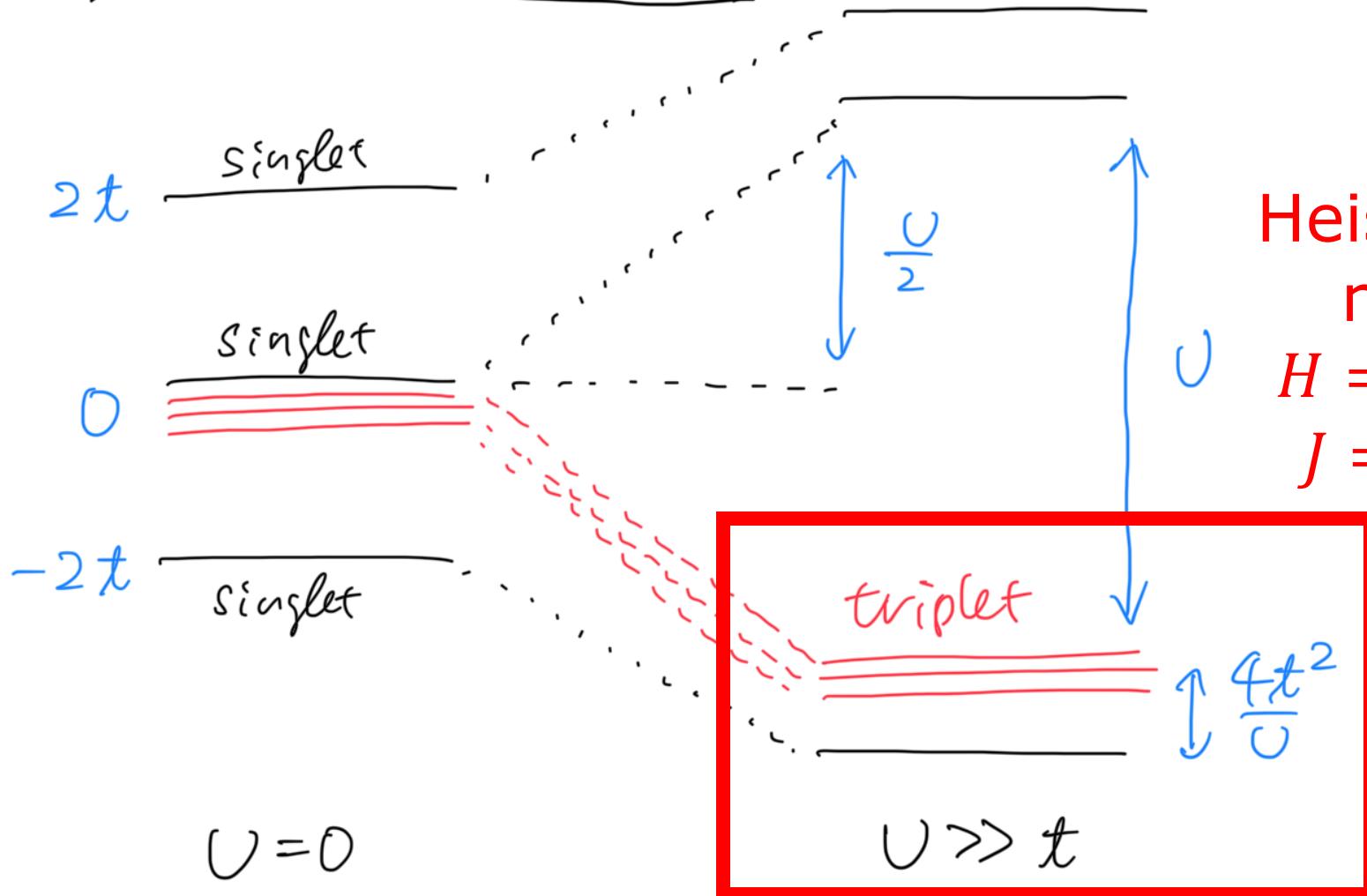
$$E = \frac{U}{2}, \pm \frac{U}{2} \sqrt{1 + \left(\frac{4t}{U}\right)^2}, -\frac{U}{2}, -\frac{U}{2}, -\frac{U}{2}$$

2-site Hubbard model



2-site Hubbard model

energy difference



Heisenberg
model
 $H = JS_1 \cdot S_2$
 $J = 4t^2/U$

Today's summary

- Brief review of itinerant electron systems
 - Electrons in crystals
 - Second quantization
 - Hubbard models
 - Solving models for simple cases
 - Noninteracting and atomic limits
 - Mean-field approximation
 - Exact diagonalization (2 sites)
→ Strong coupling limit: Heisenberg model (spin system)
- Magnetism and quantum spin liquid
 - Spin models
 - Frustrated magnetism and quantum spin liquid
 - Kitaev honeycomb spin liquid