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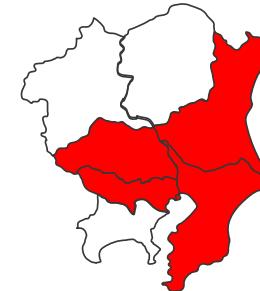
Condensed matter physics: from magnetism to quantum spin liquid I

Sophia University Ryui Kaneko (金子隆威)

https://github.com/ryuikaneko/lecturenote_2024_condmat

Self introduction

- Ryui Kaneko (金子 隆威)
 - Born in Tokyo, raised in Saitama
- Academic career
 - 2009 Tokyo Institute of Technology [bachelor]
 - 2011 Tokyo University [master]
 - 2014 Tokyo University [doctor]
 - 2014-2023 Goethe University (Germany), NIMS, ISSP, Kindai University [postdoc]
 - 2023 Waseda University [associate professor]
 - 2024 Sophia University [associate professor]
- Research interest
 - CondMat, StatMech, ComputationalPhys, ...
 - Magnetism, spin liquid, superconductivity, critical phenomena, tensor network, variational Monte Carlo, ...



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

How to describe everything for our everyday world

The Theory of Everything

R. B. Laughlin* and David Pines^{†‡§}

Except cosmology, general relativity,
particle physics, ...

*Department of Physics, Stanford University, Stanford, CA 94305; [†]Institute for Complex Adaptive Matter, University of California Office of the President, Oakland, CA 94607; [‡]Science and Technology Center for Superconductivity, University of Illinois, Urbana, IL 61801; and [§]Los Alamos Neutron Science Center Division, Los Alamos National Laboratory, Los Alamos, NM 87545

Contributed by David Pines, November 18, 1999

The Theory of Everything is a term for the ultimate theory of the universe—a set of equations capable of describing all phenomena that have been observed, or that will ever be observed (1). It is the modern incarnation of the reductionist ideal of the ancient Greeks, an approach to the natural world that has been fabulously successful in bettering the lot of mankind and continues in many people's minds to be the central paradigm of physics. A special case of this idea, and also a beautiful instance of it, is the equation of conventional nonrelativistic quantum mechanics, which describes the everyday world of human beings—air, water, rocks, fire, people, and so forth. The details of this equation are less important than the fact that it can be written down simply and is completely specified by a handful of known quantities: the charge and mass of the electron, the charges and masses of the atomic nuclei, and Planck's constant. For experts we write

$$i\hbar \frac{\partial}{\partial t} |\Psi\rangle = \mathcal{H}|\Psi\rangle \quad [1]$$

where

$$\begin{aligned} \mathcal{H} = & - \sum_j^{N_e} \frac{\hbar^2}{2m} \nabla_j^2 - \sum_\alpha^{N_i} \frac{\hbar^2}{2M_\alpha} \nabla_\alpha^2 \\ & - \sum_j^{N_e} \sum_\alpha^{N_i} \frac{Z_\alpha e^2}{|\vec{r}_j - \vec{R}_\alpha|} + \sum_{j \ll k}^{N_e} \frac{e^2}{|\vec{r}_j - \vec{r}_k|} + \sum_{\alpha \ll \beta}^{N_i} \frac{Z_\alpha Z_\beta e^2}{|\vec{R}_\alpha - \vec{r}_\beta|}. \end{aligned} \quad [2]$$

The symbols Z_α and M_α are the atomic number and mass of the α^{th} nucleus, R_α is the location of this nucleus, e and m are the electron charge and mass, r_j is the location of the j^{th} electron, and \hbar is Planck's constant.

Less immediate things in the universe, such as the planet Jupiter, nuclear fission, the sun, or isotopic abundances of elements in space are not described by this equation, because important elements such as gravity and nuclear interactions are missing. But except for light, which is easily included, and possibly gravity, these missing parts are irrelevant to people-scale phenomena. Eqs. 1 and 2 are, for all practical purposes, the Theory of Everything for our everyday world.

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, ...

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

spin and charge degrees of freedom

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



Heisenberg model

spin degrees of freedom

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



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, ...

Rough outline

Hamiltonian for electrons in atoms

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Second quantization

Hubbard model

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

References

- A. L. Fetter, J. D. Walecka, Quantum Theory of Many-Particle Systems
- F. H. L. Essler et al., The One-Dimensional Hubbard Model
- Sebastian Will, PhD thesis, <https://www.physics.utoronto.ca/~jht/pub/theses/Will2011.pdf>
- Autumn School on Correlated Electrons: Simulating Correlations with Computers 20-24 September 2021, <https://www.cond-mat.de/events/correl21/manuscripts/correl21.pdf>
- 猪木慶治, 川合光, 量子力学1・2
- 今田正俊, 統計物理学

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 $|n_\alpha\rangle$

State at position r single electron in state α

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

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

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

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

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

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

Conversely,

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

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

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

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 : $H\psi_\alpha(r) = E_\alpha \psi_\alpha(r)$

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

Then,

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

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)

Hamiltonian in crystals

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:

$$\hat{H} = - \sum_{ij\sigma} t_{ij\sigma} \hat{c}_{i\sigma}^+ \hat{c}_{j\sigma} + \sum_{ijkl} V_{ijkl} \sum_{\sigma\sigma'} \hat{c}_{i\sigma}^+ \hat{c}_{j\sigma}^+ \hat{c}_{k\sigma'} \hat{c}_{l\sigma}$$

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

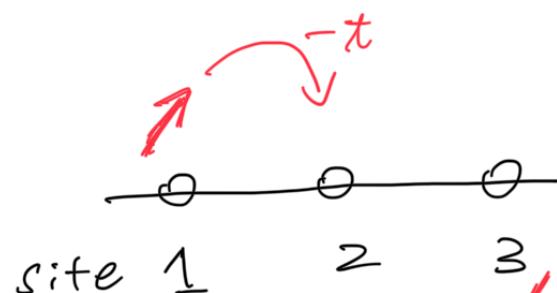
$$\hat{H} = -t \sum_{\langle i,j \rangle} (\hat{c}_{i\sigma}^+ \hat{c}_{j\sigma} + \hat{c}_{j\sigma}^+ \hat{c}_{i\sigma})$$

$\langle \cdot \rangle$ denotes nearest neighbors

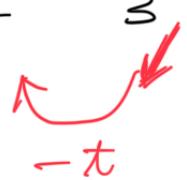
$$+ U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

Hubbard model

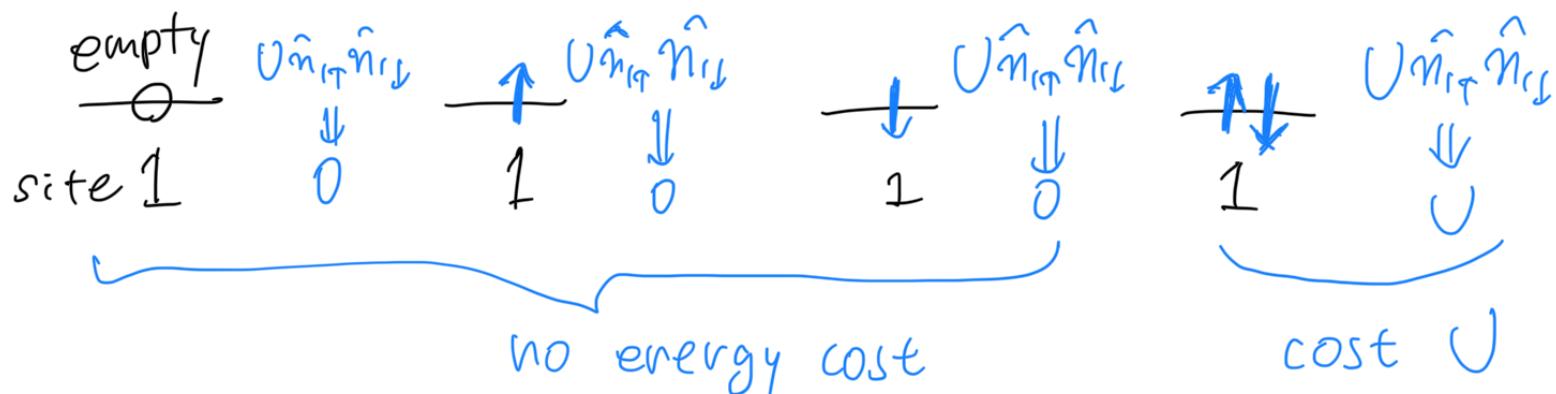
$$\hat{H} = - \sum_{i,j,\sigma} t_{ij} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \sum_i U_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$



$$-t \hat{c}_{2\uparrow}^\dagger \hat{c}_{1\uparrow}$$



$$-t \hat{c}_{2\downarrow}^\dagger \hat{c}_{3\downarrow}$$



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, ...

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 ($U=0$)

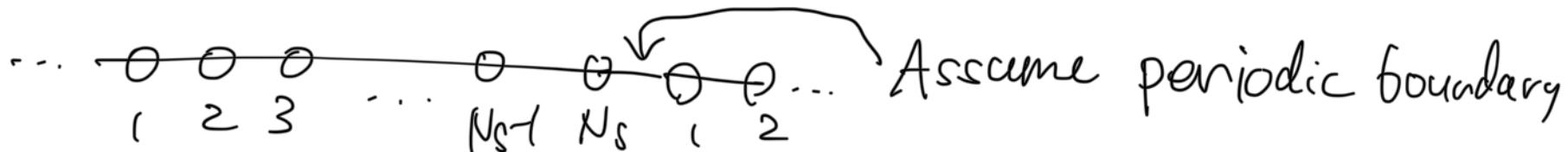
$$\hat{H} = -t \sum_{\langle i,j \rangle} (\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \hat{c}_{j\sigma}^\dagger \hat{c}_{i\sigma})$$

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,

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



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

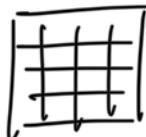
$$\hat{H} = -t \sum_k (e^{ik} + e^{-ik}) \hat{c}_{k\sigma}^\dagger \hat{c}_{k\sigma} = \sum_k \epsilon_k \hat{c}_k^\dagger \hat{c}_k$$

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

Noninteracting limit ($U=0$)

1D 

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

2D 

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

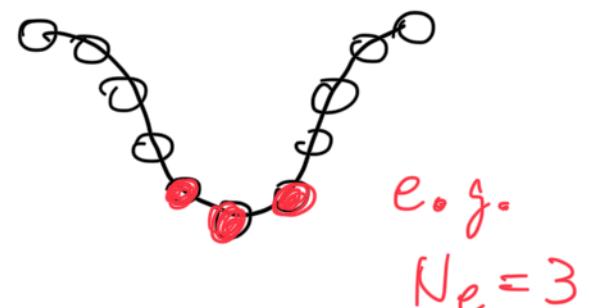
3D 

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

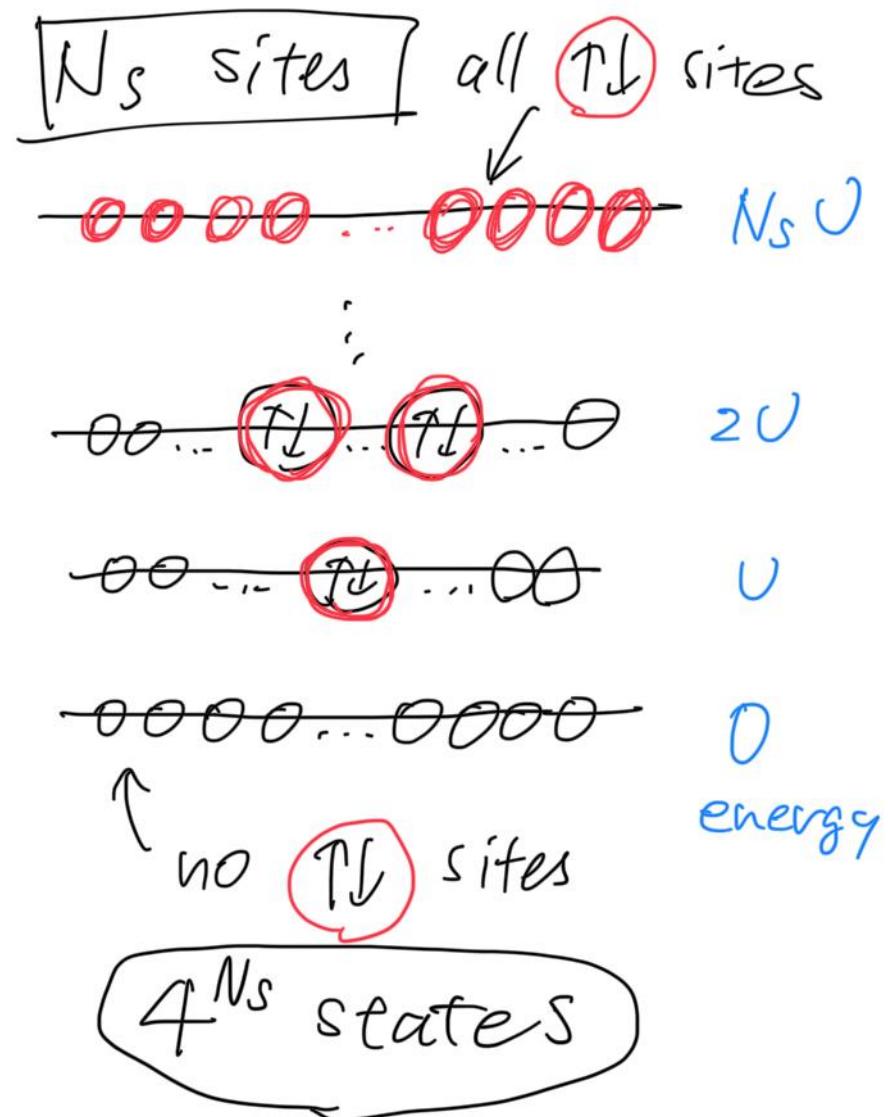
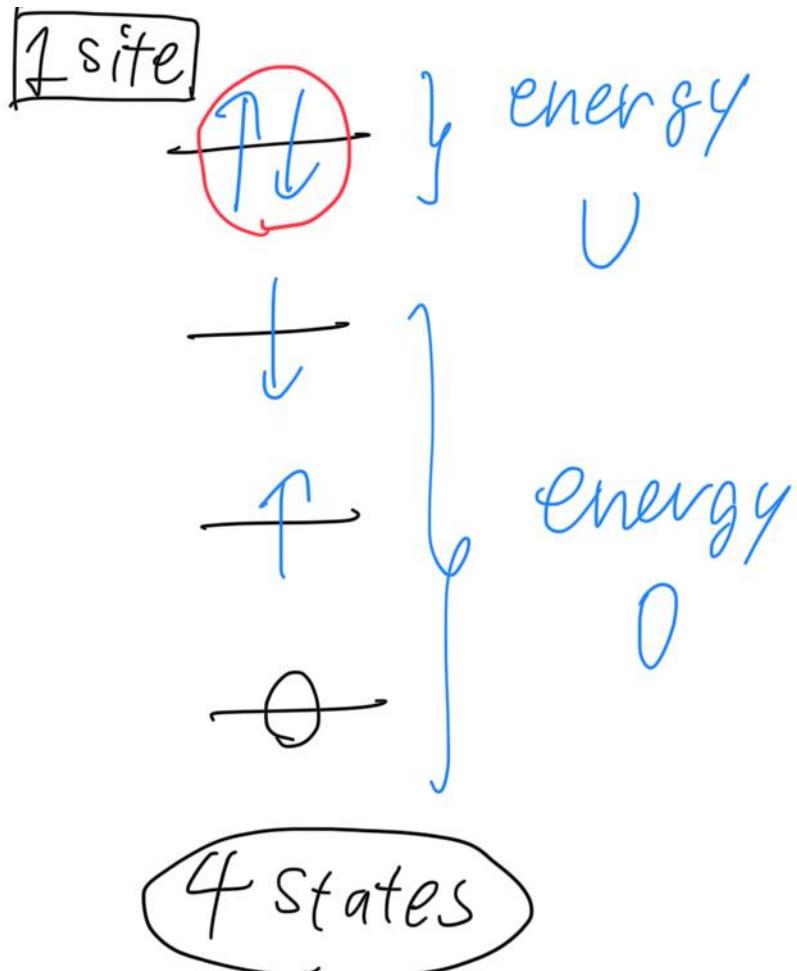
⋮

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

- $U=0$ 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)

Mean-field (MF) approximation

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

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

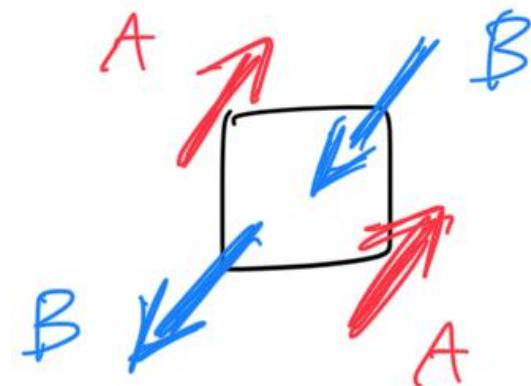
$$\begin{aligned} &= \langle \hat{A} \rangle \langle \hat{B} \rangle + \langle \hat{A} \rangle (\hat{B} - \langle \hat{B} \rangle) + (\hat{A} - \langle \hat{A} \rangle) \langle \hat{B} \rangle \\ &\quad + (\hat{A} - \langle \hat{A} \rangle) (\hat{B} - \langle \hat{B} \rangle) \quad \text{Throw away fluctuations!}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

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

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

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

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

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

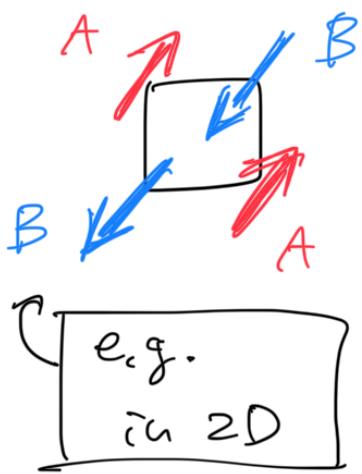
$$\sim \sum_k \varepsilon_k \hat{c}_{k\uparrow}^+ \hat{c}_{k\downarrow} \quad \text{Fourier transform}$$

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



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

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

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

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

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

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

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

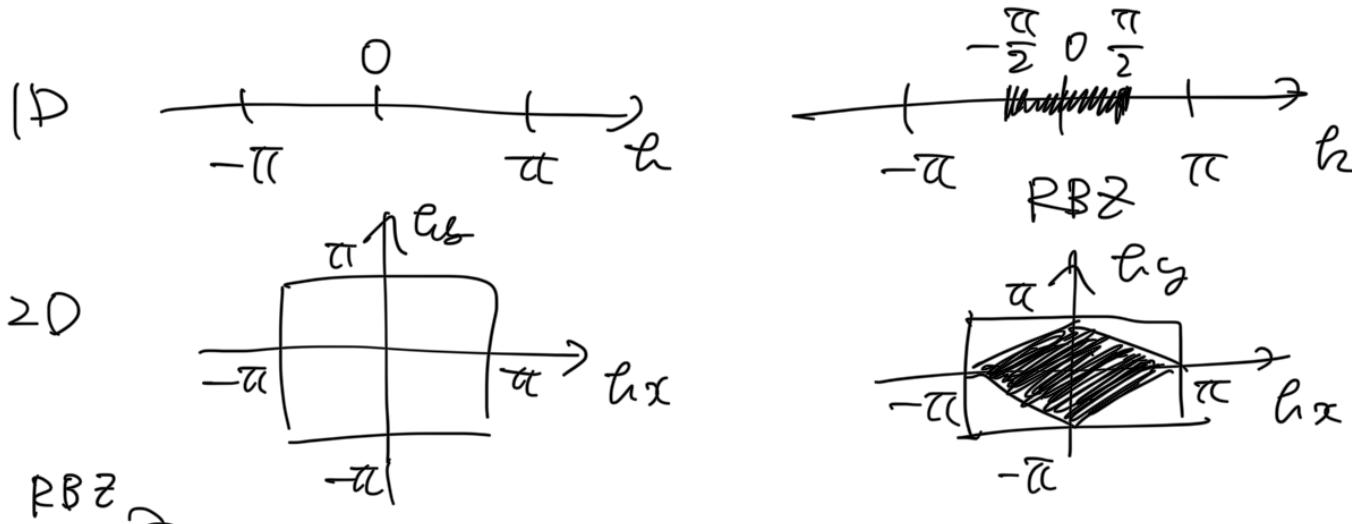
We have

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

(up to constant terms)

Mean-field (MF) approximation

Rewrite sum by reduced Brillouin zone (RBZ)



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

Mean-field (MF) approximation

$$H \sim \sum_{\sigma} \begin{pmatrix} C_{\sigma\sigma} & C_{\sigma-\alpha\sigma} \\ C_{\sigma\alpha\sigma} & C_{\sigma-\alpha\sigma} \end{pmatrix}$$
$$\begin{pmatrix} E_h + \frac{U}{2} & -Um \\ -Um & E_{h-\alpha} + \frac{U}{2} \end{pmatrix} \begin{pmatrix} C_{\sigma\sigma} \\ C_{\sigma-\alpha\sigma} \end{pmatrix}$$
$$\sigma = \begin{cases} + & \text{for } \uparrow \\ - & \text{for } \downarrow \end{cases}$$

After diagonalizing the 2×2 matrix, we have

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

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

Mean-field (MF) approximation

Magnetization can be obtained from
self-consistent equation

$$m = \frac{1}{N_s} \sum_{i\sigma} \langle n_{i\sigma} \rangle = \frac{1}{N_s} \sum_{i\sigma} \langle c_{i\sigma}^\dagger c_{i\sigma} \rangle$$

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

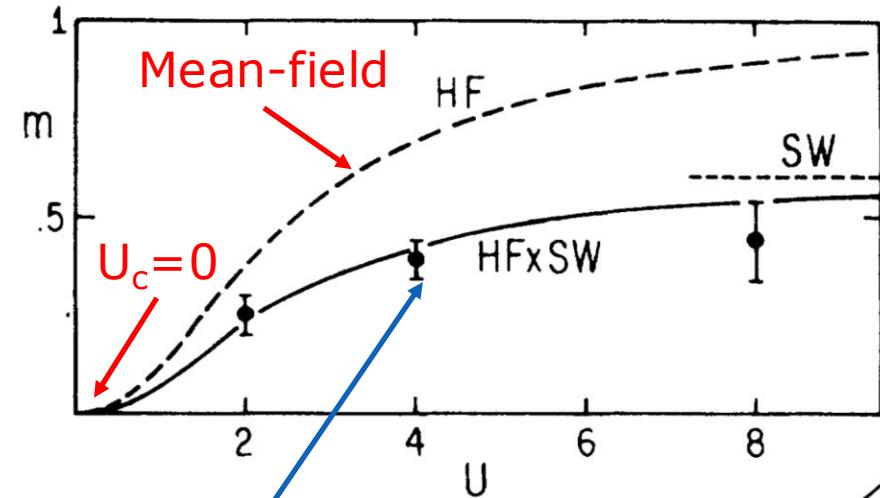
$$I = U \int \frac{d^D k}{(2\pi)^D} \frac{1}{\sqrt{\epsilon_k^2 + U^2 m^2}}$$

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

Density of states in hypercubic systems

Transition occurs at $U_c = 0$

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



Numerically exact
(quantum Monte Carlo)

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

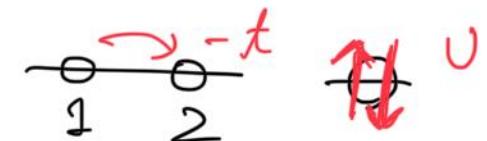
J. E. Hirsch and S. Tang, PRL.62.591('88)

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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

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

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

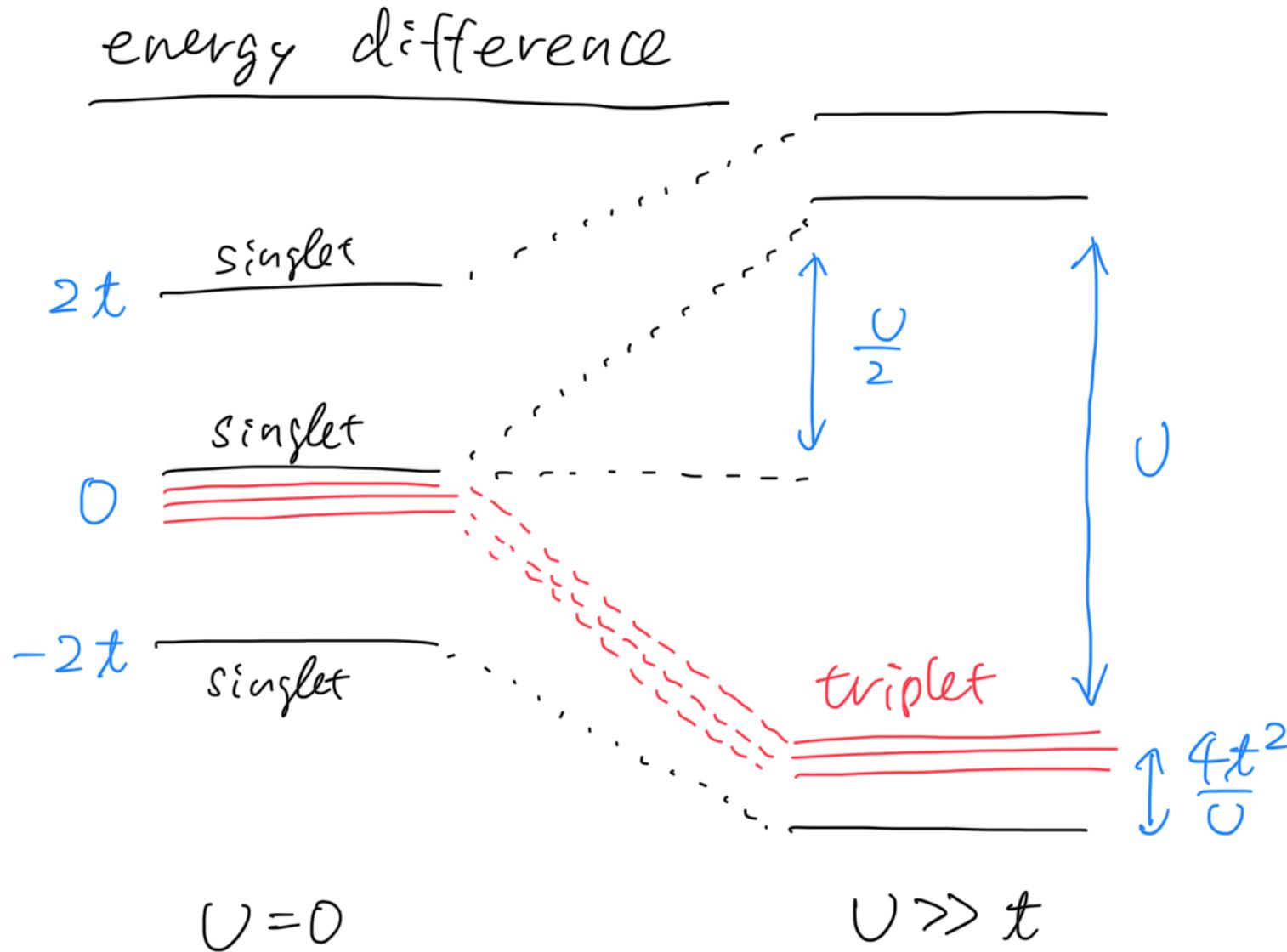
3x3 matrix for singlet states

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

block diagonalized for triplet states

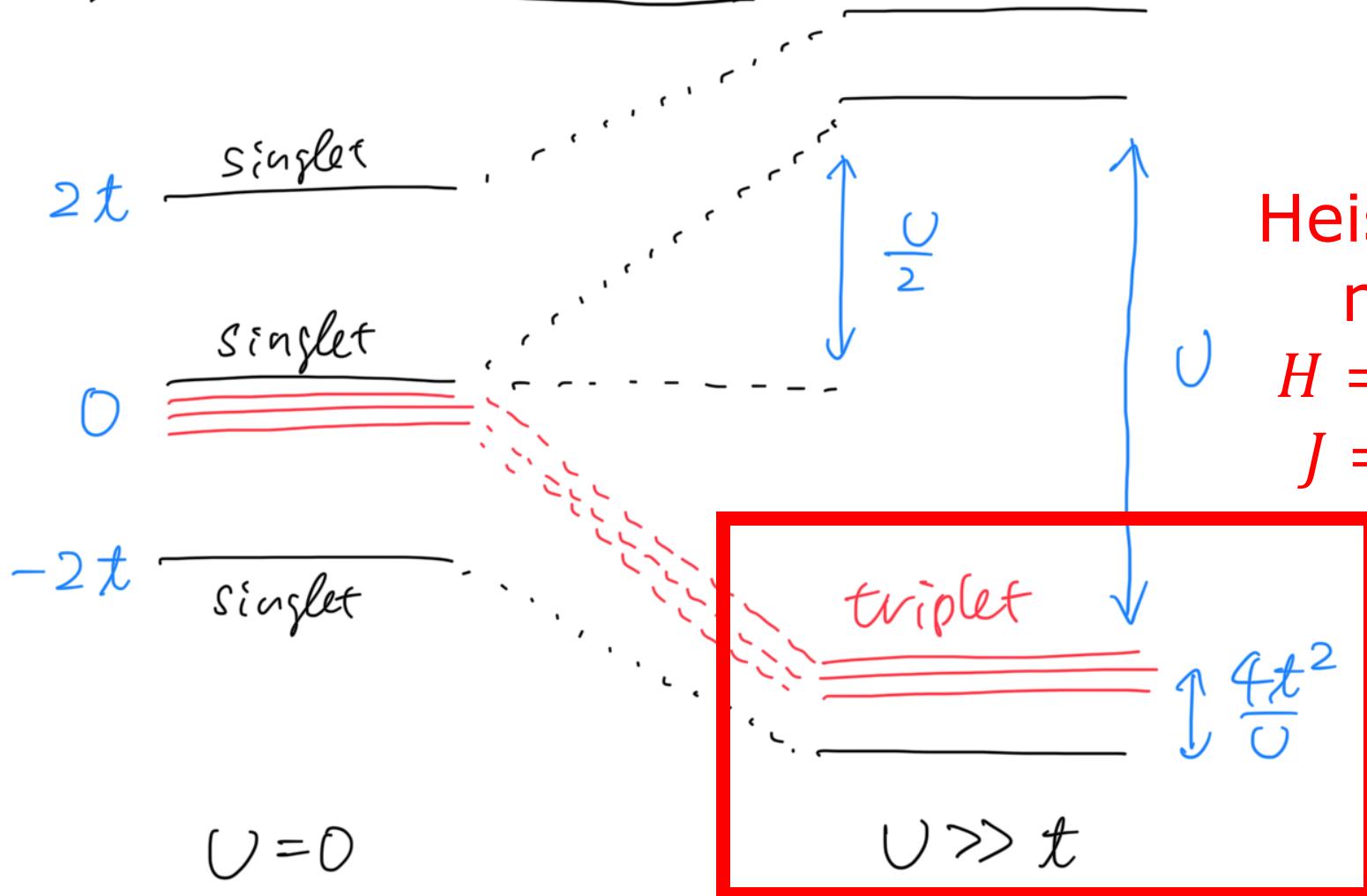
$$E = \frac{U}{2}, \pm \frac{U}{2} \sqrt{1 + \left(\frac{4t}{U}\right)^2}, -\frac{U}{2}, -\frac{U}{2}, -\frac{U}{2}$$

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

https://github.com/ryuikaneko/lecturenote_2024_condmat