

Introduction

Magnetic Moment
Magnetic Ordering
Origin of Magnetism

Origin of Magnetism

- Let's consider magnetic moments in an external magnetic field $\vec{B}(\vec{H})$
- Magnetization (Boltzmann distribution):

$$\vec{p} \rightarrow \vec{p} - \frac{e}{c} \vec{A}$$

$$H = \sum_i \frac{1}{2\mu_i} \left(\vec{p}_i - \frac{e}{c} \vec{A} \right)^2 + \sum_i e\phi_i - \sum_i \vec{B} \cdot \vec{m}_i$$

$$\vec{M} = \frac{N}{V} \langle \vec{m} \rangle = \frac{N}{V} \frac{1}{Z} \int \dots \int \prod_i \vec{m}_i d\vec{q}_i d\vec{p}_i e^{-\beta H} = - \frac{N}{V} \frac{\partial \ln Z}{\partial \vec{B}}$$

Origin of Magnetism

- Change variables

$$\vec{u}_i = \vec{p}_i - \frac{e}{c} \vec{A} \quad \rightarrow \quad Z = \int \dots \int \prod_i d\vec{q}_i d\vec{u}_i e^{-\beta H}$$

(Integration from $-\infty$ to $+\infty$), Z is independent of A , so its derivative with respect to magnetic field is zero, i.e., $\overrightarrow{M} = 0$ (*Miss van Leeuwen's Theorem*)

- Conclusion: we have to consider the discreteness of the eigenvalues of the system, i.e., **quantum nature**.

Physical Issues

- There are many
- Why/how the nature creates these ordered structures? (QM, microscopic)
- Order \leftrightarrow Disorder Transition
(thermodynamic properties, macroscopic)
- Dynamics of carriers
- Relation to other quantum state?
- ...

Microscopic Mechanisms

- ⊕ Stoner criterion
- ⊕ Band structures (van Hove, Flat-band, etc.)
- ⊕ Itinerant versus localization
- ⊕ The role of electron-electron interaction
($U=\infty$)
- ⊕ The role of degeneracy (multi-orbital systems)
- ⊕ ...

The Hubbard Model

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Outline

- ⊕ Model Hamiltonian
- ⊕ History
- ⊕ Current Interest
- ⊕ Related Models
- ⊕ Symmetries
- ⊕ Solving Many-Body Hamiltonian

Hubbard Model

Electron correlations in narrow energy bands

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It is pointed out that one of the main effects of correlation phenomena in d - and f -bands is to give rise to behaviour characteristic of the atomic or Heitler-London model. To investigate this situation a simple, approximate model for the interaction of electrons in narrow energy bands is introduced. The results of applying the Hartree-Fock approximation to this model are examined. Using a Green function technique an approximate solution of the correlation problem for this model is obtained. This solution has the property of reducing to the exact atomic solution in the appropriate limit and to the ordinary uncorrelated band picture in the opposite limit. The condition for ferromagnetism of this solution is discussed. To clarify the physical meaning of the solution a two-electron example is examined.

Proc. R. Soc. London, Ser. A276, 283(1963); 281, 401 (1964). **7844 citations (May, 2019)**

Hubbard Model



$$H = - \sum_{i,j,\sigma=\uparrow\downarrow} t_{i,j} c_{i\sigma}^+ c_{j\sigma} + \frac{1}{2} \sum_{i,j,l,m,\sigma,\sigma'} U_{ij,lm} c_{i\sigma}^+ c_{j\sigma'}^+ c_{l\sigma'} c_{m\sigma}$$

where $U_{ij,lm} = \int d\mathbf{r}_1 d\mathbf{r}_2 \Psi_i^*(\mathbf{r}_1) \Psi_j^*(\mathbf{r}_2) U(\mathbf{r}_1 - \mathbf{r}_2) \Psi_l(\mathbf{r}_2) \Psi_m(\mathbf{r}_1)$

$t_{i,j} = \int d\mathbf{r} \Psi_i^*(\mathbf{r}) \Delta(\mathbf{r}) \Psi_j(\mathbf{r})$

Coulomb potential

- ✿ **Hubbard approximation (1963):**

$t_{i,j} = t$ if i and j are nearest neighbor

$U_{ij,lm} = U \delta_{ij} \delta_{il} \delta_{im}$, (on-site U only).

- ✿ **Extended Hubbard model:** $U_{ij,lm} = V \delta_{ij} \delta_{jl} \delta_{i,j \pm \mathbf{a}}$.
- ✿ **Magnetism.**

Why the Hubbard Model?

- ⊕ *Simplest model to describe many-body interactions.*
- ⊕ Some Statistics: (Web of Science)
“Hubbard” before 1987: 930/937; 1987-2011:
5,243/15,702
- ⊕ Widely used in condensed matter physics:
 - Quasi-2D organic superconductor
 - 1D conducting polymers, the Peierls-Hubbard model
 - Metal-insulator transition
 - Degenerate Hubbard model
 - LDA + U
 - Books, Meetings (e.g., APS Hubbard Section, etc.)
 - ...

Hubbard Model

$$H_{\text{Hubbard}} = -t \sum_{\langle i,j \rangle \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

Kinetic
Coulomb

- $H_k = \sum_{k\sigma} \varepsilon_k c_{k\sigma}^\dagger c_{k\sigma}$

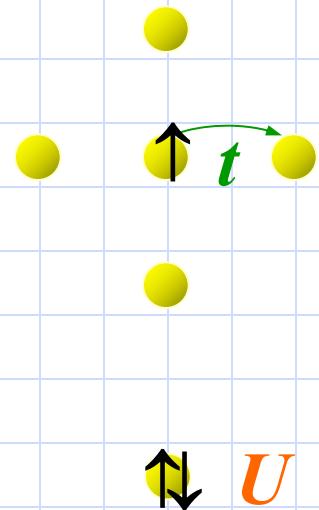
$$\varepsilon_k = \sum_{i=1}^D -2t \cos k_i \quad (\text{Bipartite lattice})$$

$$W = 4Dt \quad D : \text{dimensionality}$$

- $H_I = \sum_i (-2U/3)(\mathbf{S}_i)^2 + N_e U/6$

- Parameters: $U/t, N_e/N$

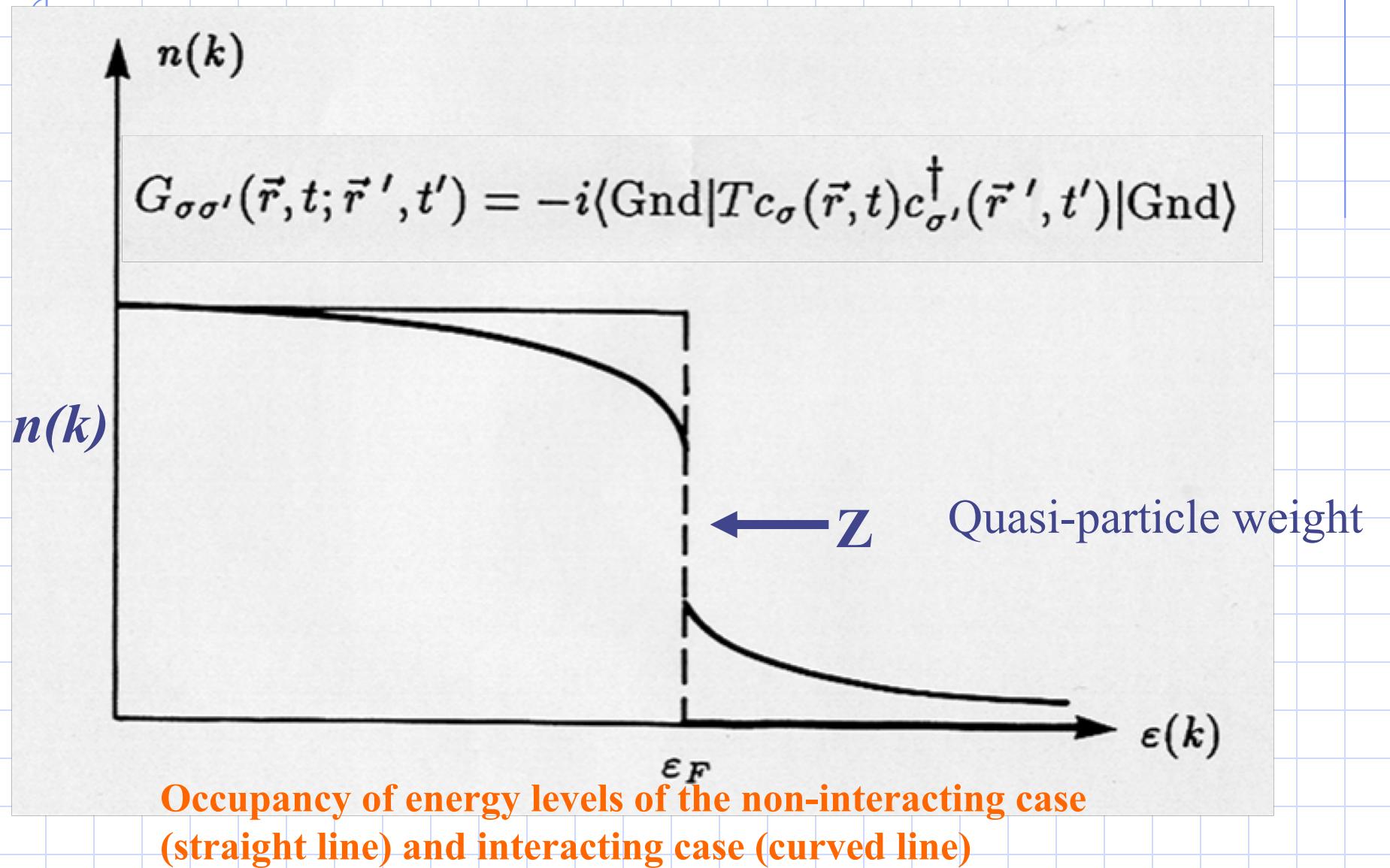
Localized moment



Current Interests

- *Superconductivity:*
 - High- T_c superconductors
 - Organic superconductors
- $n(k), Z_?$, is 2D close to 1D?
- Spin-charge separation
- Magnetism
- Phase separation
- Effects of long-range Coulomb interactions
- Emulations in other realms: Atomic Physics
 - Cold atoms trapped by laser beams
- Out-of-equilibrium

Green's Function



Models for Highly Correlated Systems

- Three-band Hubbard Model (Cu-O cuprates)
- Degenerate Hubbard Model (d or f -orbital)
- Peierls-Hubbard Model (lattice distortion)
- Anderson Impurity/Lattice Model (local moment)
- Kondo Impurity/Lattice Model
- Double Exchange Model (CMR materials)
- Quantum Spin Model (e.g., Heisenberg Model)
- ...

3-Band Hubbard Model

$$\varepsilon = \varepsilon_p - \varepsilon_d = 3.6 \text{ eV}$$

$$t_{pd} = 1.3 \text{ eV}$$

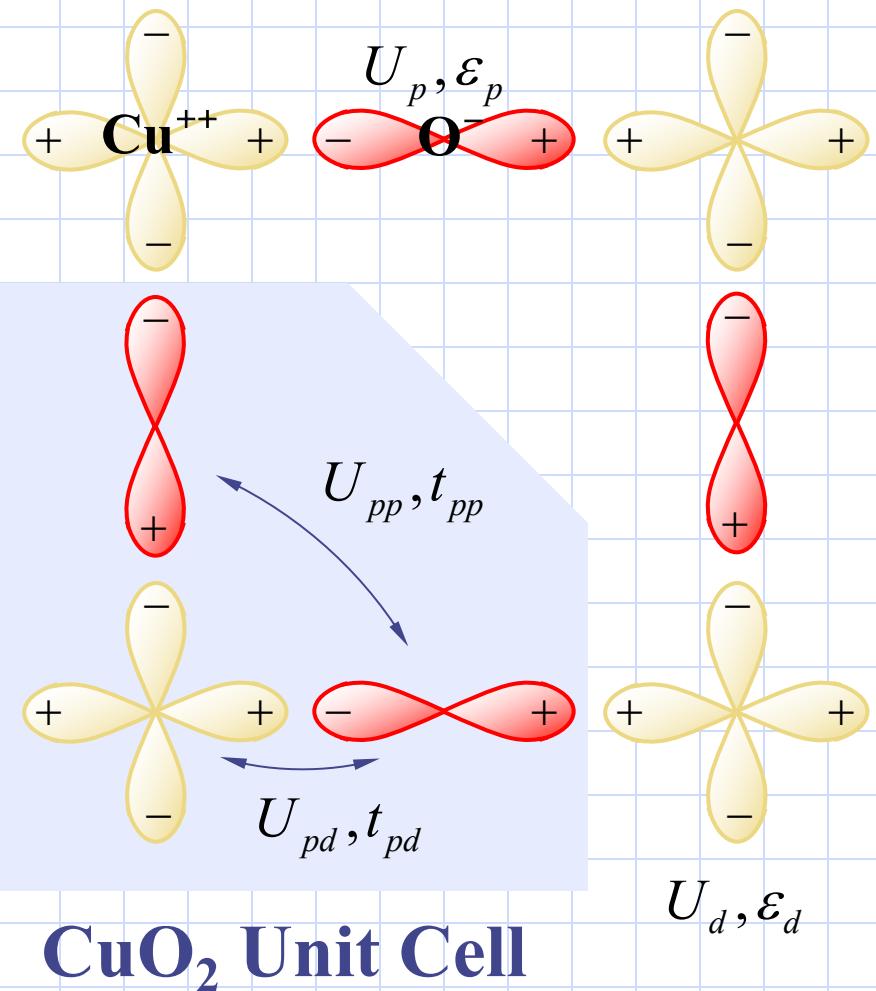
$$t_{pp} = 0.65 \text{ eV}$$

$$U_d = 10.5 \text{ eV}$$

$$U_p = 4 \text{ eV}$$

$$U_{pd} = 1.2$$

LDA Estimates



The Peierls-Hubbard Model

$$H = H_{\text{electron}} + H_{\text{phonon}} + H_{\text{electron-phonon}}$$

$$H_{\text{electron}} = -t \sum_{\langle i,j \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + H.c) + \sum_i U_i n_{i\uparrow} n_{i\downarrow} + V \sum_{\langle i,j \rangle} n_i n_j \\ + \sum_{i\sigma} \varepsilon_i n_{i\sigma} + \sum_i (-1)^i h_s (n_{i\uparrow} - n_{i\downarrow})$$

$$H_{\text{phonon}} = \sum_i \left(\frac{p_i^2}{2m} + \frac{1}{2} K_1 q_i^2 + \frac{1}{4} g_1 q_i^4 \right) + \sum_i \frac{P_i^2}{2M} + \sum_{\langle i,j \rangle} \left(\frac{1}{2} K_2 u_{ij}^2 + \frac{1}{4} g_2 u_{ij}^4 \right)$$

$$H_{\text{electron-phonon}} = \lambda_1 \sum_{i\sigma} q_i n_{i\sigma} + \lambda_2 \sum_{\langle i,j \rangle, \sigma} u_{ij} (c_{i\sigma}^\dagger c_{j\sigma} + H.c)$$

where $n_i = n_{i\uparrow} + n_{i\downarrow}$

u_{ij} = Relative Lattice Displacement on Bond $\langle i, j \rangle$

q_i = Optical Phonon

SSH, Holstein (Dimerization, Soliton, etc).

Adiabatic Approximation (Double Well)

The Degenerate Hubbard Model

$$\begin{aligned}\hat{H} = & \sum_{\langle i,j \rangle, \sigma} \sum_{m,m'} t_{m,m'} \left(\hat{c}_{i,m,\sigma}^\dagger \hat{c}_{j,m',\sigma} + h.c. \right) \\ & + \sum_{i,m} U \hat{n}_{i,m,\uparrow} \hat{n}_{i,m,\downarrow} + \sum_{i,\sigma,\sigma'} V \hat{n}_{i,1,\sigma} \hat{n}_{i,2,\sigma'} \\ & - \sum_{i,\sigma,\sigma'} J \hat{c}_{i,1,\sigma}^\dagger \hat{c}_{i,1,\sigma'} \hat{c}_{i,2,\sigma'}^\dagger \hat{c}_{i,2,\sigma}\end{aligned}$$

- Consider degenerate d -orbital in real metals.
- Hund's rule couplings
- Ferromagnetism?

Proc. R. Soc. London, Ser. A276, 283(1963); 281, 401 (1964).

The Anderson Impurity Model

$$\begin{aligned}\hat{H} = & \sum_{\langle i,j \rangle, \sigma} t_{ij} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \sum_{\sigma} \varepsilon_f \hat{n}_{f,\sigma} + U \hat{n}_{f,\uparrow} \hat{n}_{f,\downarrow} \\ & + \sum_{i,\sigma} \left(V_j \hat{f}_\sigma^\dagger \hat{c}_{i,\sigma} + V_j^* \hat{c}_{i,\sigma}^\dagger \hat{f}_\sigma \right) \quad \text{← Hybridization}\end{aligned}$$

- Used to describe magnetic impurities embedded in metals.
- Anderson lattice model

Kondo model (intimately related to the Anderson impurity model, as can be shown by Schrieffer–Wolff transformation.)

Local moments and localized states

P. W. Anderson

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I was cited for work both in the field of magnetism and in that of disordered systems, and I would like to describe here one development in each field which was specifically mentioned in that citation. The two theories I will discuss differed sharply in some ways. The theory of local moments in metals was, in a sense, easy: it was the condensation into a simple mathematical model of ideas which were very much in the air at the time, and it had rapid and permanent acceptance because of its timeliness and its relative simplicity. What mathematical difficulty it contained has been almost fully cleared up within the past few years.

Localization was a different matter: very few believed it at the time, and even fewer saw its importance; among those who failed to fully understand it at first was certainly its author. It has yet to receive adequate mathematical treatment, and one has to resort to the indignity of numerical simulations to settle even the simplest questions about it. Only now, and through primarily Sir Nevill Mott's efforts, is it beginning to gain general acceptance.

Yet these two finally successful brainchildren have also much in common: first, they flew in the face of

require an additional excitation energy U , the energy necessary to change the configurations of two distant atoms from $d^n + d^n$ to $d^{n-1} + d^{n+1}$. This energy U is essentially the Coulomb repulsive energy between two electrons on the same site, and can be quite large (see Fig. 1). To describe such a situation, I set up a model Hamiltonian (now called the "Hubbard" Hamiltonian).

$$H = \sum_{i,j,\sigma} b_{ij} c_{i\sigma}^+ c_{j\sigma} + \sum_i U n_{i\uparrow} n_{i\downarrow}. \quad (1)$$

Here b_{ij} represents the amplitude for the electron to "hop" from site to site—such hops as shown in Fig. 1, right half; and U represents the repulsion energy between two opposite spin electrons on the same site (parallel, of course, being excluded). With Eq. (1)—appropriately generalized—it was possible to understand the predominantly antiferromagnetic interactions of the spins in these Mott insulators, which include the ancient "lodestone" or magnetite, as well as the technically important garnets and ferrites. These interactions are caused by the virtual hopping of electrons from a site to its neighbor and return, which is only possible for antiferromagnetism, where the requisite

Citations from P. W. Anderson

Nobel Prize (1977) Speech

- I was cited for both in the field of magnetism and in that of disordered systems.
- To describe such a situation, I set up a model Hamiltonian (now called the “Hubbard” Hamiltonian)

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

Solution of the Hubbard Model

- ⊕ In one dimension:
 - Lieb-Wu Bethe Ansatz solution (1968)
 - Field theory
 - RG analysis
 - ...
- ⊕ For two and higher dimensions:
 - Various approximation schemes
 - Numeric: Exact diagonalization, QMC

Solving Many-Body Model Hamiltonian

- Mean-Field Approximation, Slave Particles
- Rigorous Solutions (e.g., Bethe Ansatz)
- Perturbation Theory
- Variational Wave Function
- Field Theory, Functional Integral
- Exact Diagonalization
- Quantum Monte Carlo simulations
- ...

Solving Many-Body Model Hamiltonian

- Direct Investigate H-matrix
- Canonical Transformation
- Use Symmetries
- Study Limiting Cases
- Making Approximation
- Numerical
- ...

Computational Physics does not mean “numerical”!

Solving Many-Body Model Hamiltonian

- ⊕ Direct Investigate H-matrix
 - Taking a proper basis to set up the H-matrix
 - Observe if there is any special characteristics allow us to estimate its spectrum
- ⊕ Canonical Transformation: map the model into the one we know how to solve. e.g.,
 - Fourier transform
 - Jordan-Wigner Transformation (see note), fermion \Leftrightarrow spin \Leftrightarrow boson

Symmetries in the Hubbard Model

- Gauge symmetry (charge conservation)

$$\hat{c}_{x,\sigma}^\dagger \rightarrow e^{i\alpha} \hat{c}_{x,\sigma}^\dagger \quad \text{and} \quad \hat{c}_{x,\sigma} \rightarrow e^{-i\alpha} \hat{c}_{x,\sigma}$$

$$\hat{H} = \sum_{j,j',\sigma} t_{jj'} \hat{c}_{j,\sigma}^\dagger \hat{c}_{j',\sigma} + \sum_j U_j \hat{c}_{j\uparrow}^\dagger \hat{c}_{j\uparrow} \hat{c}_{j\downarrow}^\dagger \hat{c}_{j\downarrow}$$

- Remains invariant if this transformation is applied

→ Therefore, the particle number $N_e = \sum_{j\sigma} \hat{c}_{j\sigma}^\dagger \hat{c}_{j\sigma}$ is conserved

Symmetries in the Hubbard Model

- Spin rotational invariance: SU(2) algebra
→ S^2 and S_z are good quantum numbers.

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

- Local spin operators (at site j):

$$\hat{S}_{\alpha,j} = \frac{1}{2} \sum_{\sigma,\sigma'} \hat{c}_{j,\sigma}^\dagger (\sigma_\alpha)_{\sigma\sigma'} \hat{c}_{j,\sigma'}, \text{ with } \alpha = x, y, z, \mathbf{S}_j = (S_{x,j}, S_{y,j}, S_{z,j})$$

- Global spin operators:

$$S_\alpha = \sum_j S_{\alpha,j}, \mathbf{S} = (S_x, S_y, S_z); S_\pm = S_x \pm iS_y; S_+ = \frac{1}{2} \sum_{\vec{n}} \hat{c}_{j\uparrow}^\dagger c_{j\downarrow}; S_- = S_+^\dagger$$

- They form an SU(2) algebra $[S_x, S_y] = iS_z$
- The Hamiltonian commutes with these operators → it possess SU(2) symmetry

Symmetries in the Hubbard Model

- Electron-Hole Transformations:

$$T_1: c_{i\sigma}^\dagger \leftrightarrow c_{i\sigma}$$

$$\begin{aligned} H(N_\uparrow, N_\downarrow, U, t) &= H(N - N_\uparrow, N - N_\downarrow, U, -t) \\ &\quad - U(N - N_\uparrow - N_\downarrow). \end{aligned}$$

$$T_2: c_{i\sigma}^\dagger \leftrightarrow (-1)^i c_{i\sigma}^\dagger$$

$$H(N_\uparrow, N_\downarrow, U, t) = H(N_\uparrow, N_\downarrow, U, -t).$$

$$T_3: c_{i\sigma}^\dagger \leftrightarrow (-1)^i c_{i\sigma}$$

$$\begin{aligned} H(N_\uparrow, N_\downarrow, U, t) &= H(N - N_\uparrow, N_\downarrow, -U, t) + U(N_\uparrow) \\ &= H(N_\uparrow, N - N_\downarrow, -U, t) + U(N_\downarrow). \end{aligned}$$

Solving the Hubbard Model

- The Hamiltonian contains two parts: T and V
- T is diagonal in momentum space
- V is diagonal in real space
- T and V do not commute \rightarrow difficulty

Bethe Ansatz Approach

$$2\pi\rho(k) = 1 + \cos k \int_{-P}^P dp \frac{8U\sigma(p)}{U^2 + 16(\sin k - p)^2}$$

$$\begin{aligned} 2\pi\sigma(p) &= \int_{-Q}^Q dk \frac{8U\rho(p)}{U^2 + 16(\sin k - p)^2} \\ &\quad - \int_{-P}^P dp' \frac{4U\sigma(p')}{U^2 + 4(p - p')^2} \end{aligned}$$

$$N_e/N = \int_{-Q}^Q dk \rho(k)$$

$$N_\uparrow/N = \int_{-p}^p dp \sigma(p)$$

$$E/N = -2t \int_{-Q}^Q dk \rho(k) \cos k$$

$$P/N = \int_{-Q}^Q dk \rho(k) k$$

- Lieb and Wu, 1968
- Exact, L or ∞
- 1D Only
- No correlation functions
- No M-I transition
- Depends on the magnetization and charge densities

Solving the Hubbard Model

- Exact Solution: Bethe Ansatz
- $t = 0$, Real space
- $U = 0$, K -space; tight binding model
- 2-site problem, (Exact Diagonalization)
- Strong Coupling Limit \Rightarrow Heisenberg Model
- Mean-Field Approach
- Functional Integral
- Quantum Monte Carlo
- Variational Wave function
- Green's Function and Feynman Diagram

Solving the Hubbard Model

- ⊕ $t = 0$, solve it in real space
- ⊕ Highly degenerate
- ⊕ Classical problem (**Atomic limit** → finding configurations and their energy is reduced to a counting problem)

Solving the Hubbard Model

- ⊕ $U = 0$, solve it in K -space (tight binding)
- ⊕ Fourier transform (canonical transform)
- ⊕ Boundary conditions

Noninteracting Fermion Ring

$$H = -t \sum c_{i\sigma}^\dagger c_{i+1,\sigma} + h.c.$$

$$= \sum \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma}$$

$$c_{\mathbf{k}\sigma} = \frac{1}{\sqrt{N}} \sum e^{i\mathbf{k}\cdot\mathbf{r}_i} c_{i\sigma}$$

$$\epsilon_{\mathbf{k}} = -2t \cos k$$

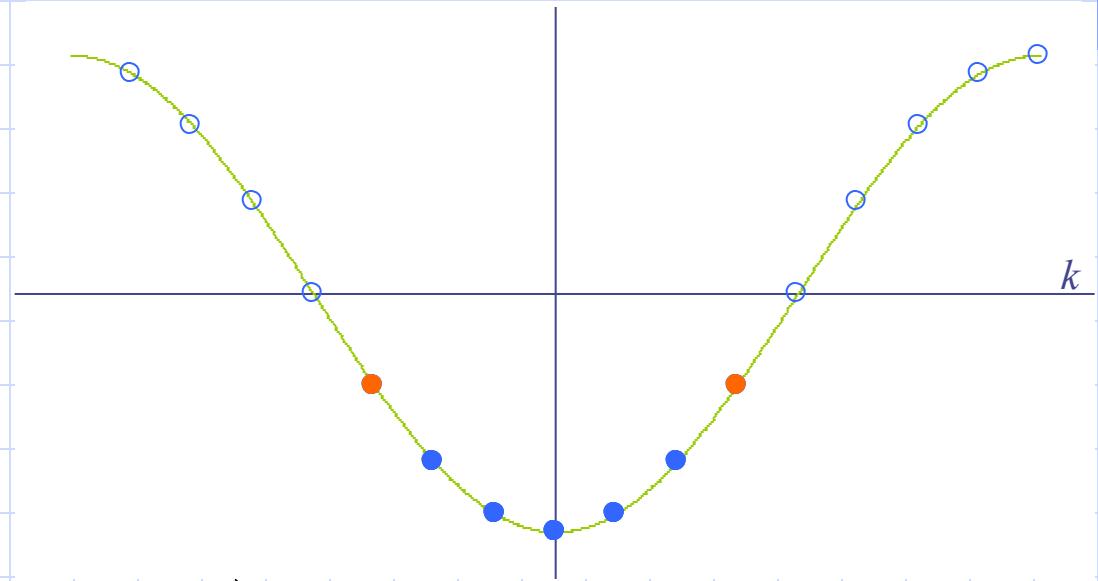
PBC

$$k = \frac{2\pi}{L} (0, \pm 1, \dots, \pm (\frac{L}{2} - 1), \frac{L}{2})$$

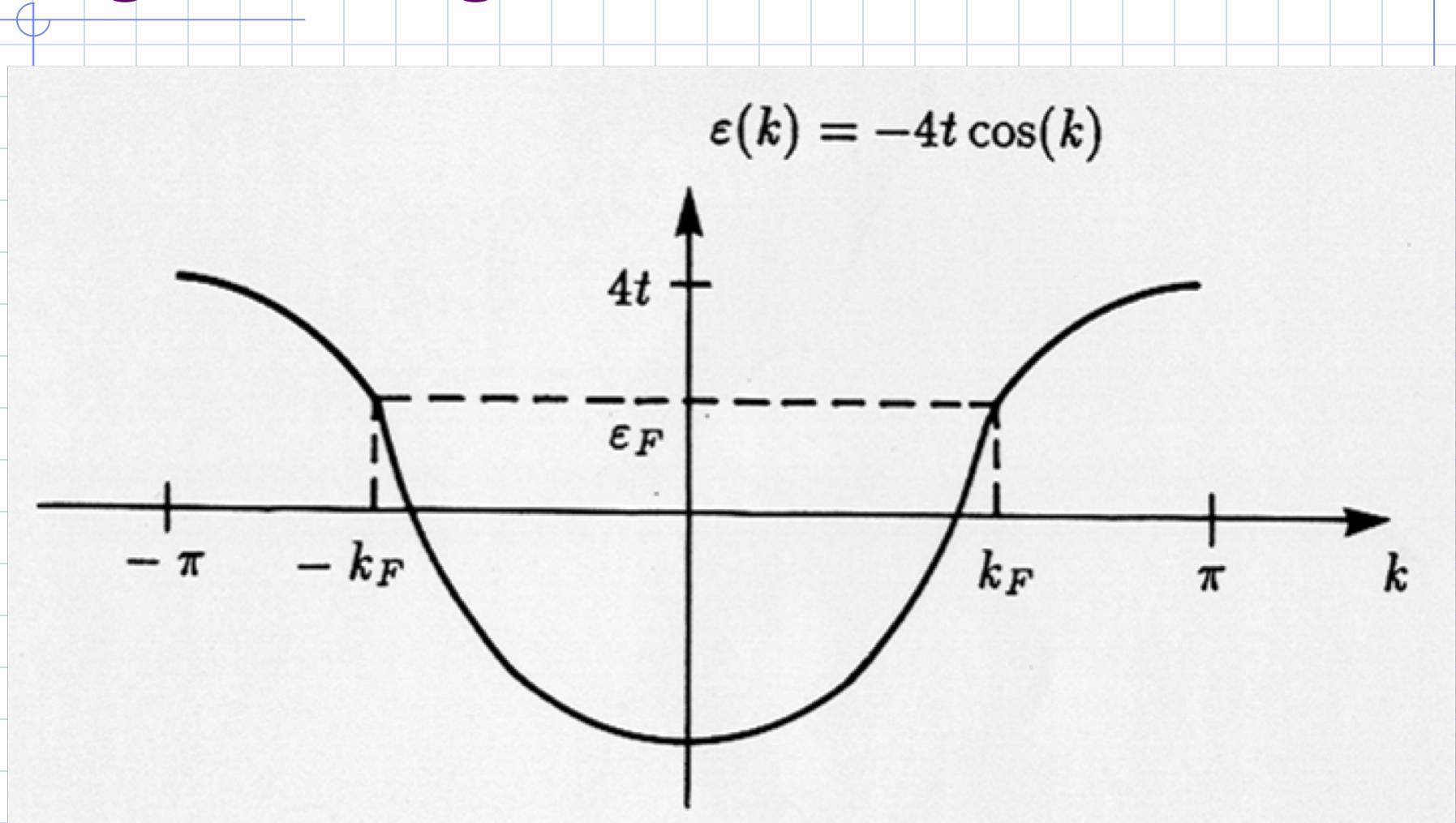
$2n + 1$: non-degenerate

$2n$: degenerate

Energy Spectrum



Tight-binding Model



Fermi Sea

- Constant energy curves for H_0 on a square lattice

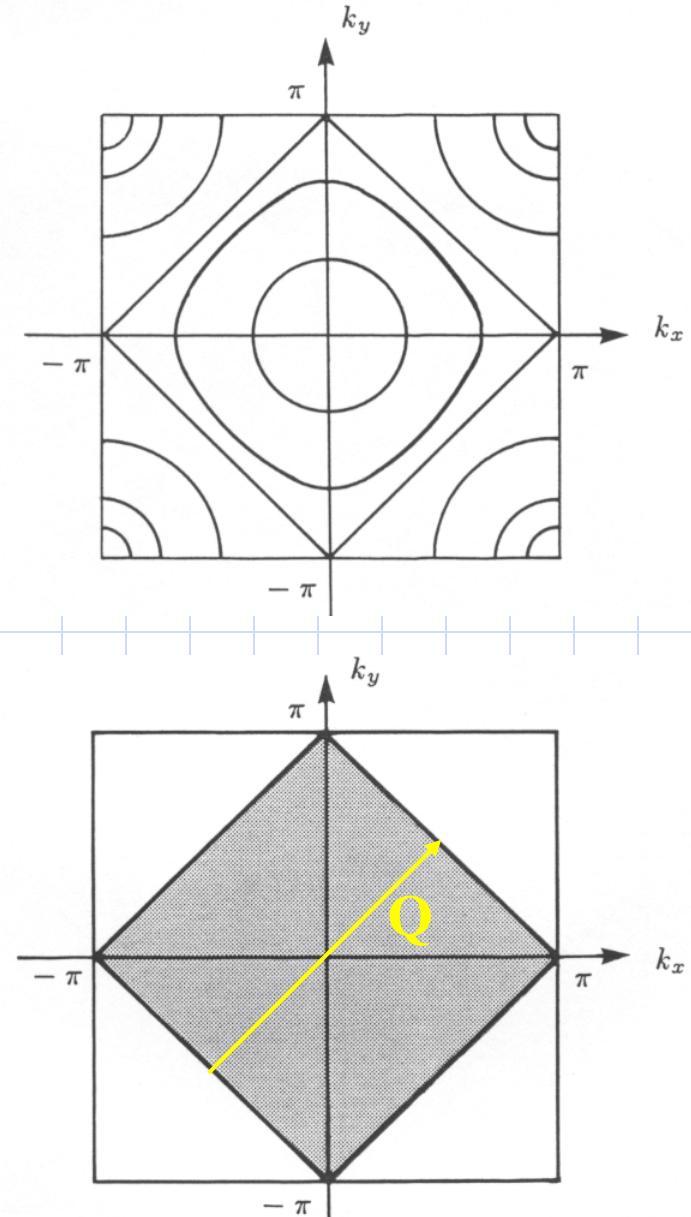
$$\epsilon_{\mathbf{k}} = -2t (\cos k_x + \cos k_y)$$

$$(-4t, 4t) \quad w = 8t$$

$$|\epsilon_{\mathbf{k}}| = \epsilon_F \quad |\epsilon_{\mathbf{k}}| < \epsilon_F$$

$$\epsilon_F = 0$$

- Fermi sea for free electrons on a square lattice at half filling (the lattice spacing is unity).



Exact Diagonalization Technique

- Set up Basis, $|i\rangle$ and H-matrix, H_{ij}
- Eigenvalue & Eigenvector: $H|\Phi\rangle = \lambda |\Phi\rangle$,
 $|\Phi\rangle = \sum_i \alpha_i |i\rangle$, ($i, j = 1, 2, \dots, M$)
- Expectations: $\langle\Phi| O |\Phi\rangle$
- Exact solution on finite size lattices
- Standard Linear Algebra Problems

Solving the Hubbard Model: 2-Site

- Model Hamiltonian

$$H = -t \sum_{\sigma} (c_{1\sigma}^\dagger c_{2\sigma} + c_{2\sigma}^\dagger c_{1\sigma}) - \mu \sum_{\sigma} (n_{1\sigma} + n_{2\sigma})$$

$$+ U(n_{1\uparrow} n_{1\downarrow} + n_{2\uparrow} n_{2\downarrow})$$

- Diagonal in particle number $N = N_{\uparrow} + N_{\downarrow}$, and magnetization $S_z = N_{\uparrow} - N_{\downarrow}$
- Symmetry with up \Leftrightarrow down, particle-hole
- $(N_{\uparrow}, N_{\downarrow}) = (0,0); (2,2)$
- $(N_{\uparrow}, N_{\downarrow}) = (1,0), (0,1); (2,1), (1,2)$
- $(N_{\uparrow}, N_{\downarrow}) = (2,0), (0,2)$
- These are easy cases to solve.

Solving the Hubbard Model: 2-Site

- $(N_\uparrow, N_\downarrow) = (1, 1)$, there are 4 configurations:

$|\uparrow, \downarrow\rangle; |\downarrow, \uparrow\rangle; |\uparrow\downarrow, \circ\rangle; |\circ, \uparrow\downarrow\rangle.$

The H -matrix is

$$\begin{pmatrix} -2\mu + U & 0 & -t & -t \\ 0 & -2\mu + U & -t & -t \\ -t & -t & -2\mu & 0 \\ -t & -t & 0 & -2\mu \end{pmatrix} \begin{pmatrix} |\uparrow\downarrow, \circ\rangle \\ |\circ, \uparrow\downarrow\rangle \\ |\uparrow, \downarrow\rangle \\ |\downarrow, \uparrow\rangle \end{pmatrix},$$

Example: making H -matrix elements

Solving the Hubbard Model: 2-Site

- Eigenvalues and Eigenvectors:

$$E_3 = -2\mu + U ,$$

$$\psi_3 = \frac{1}{\sqrt{2}}(|\uparrow\downarrow, \circ\rangle - |\circ, \uparrow\downarrow\rangle) ,$$

$$E_2 = -2\mu ,$$

$$\psi_2 = \frac{1}{\sqrt{2}}(|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle) ,$$

Easy solution

Solving the Hubbard Model: 2-Site

$$E_1 = -2\mu + \frac{1}{2}U \left[1 - \sqrt{1 + 16t^2/U^2} \right] ,$$

$$\begin{aligned}\psi_1 = & \cos\theta (| \uparrow, \downarrow \rangle + | \downarrow, \uparrow \rangle) \\ & + \sin\theta (| \uparrow\downarrow, \circ \rangle + | \circ, \uparrow\downarrow \rangle) ,\end{aligned}$$

$$E_4 = -2\mu + \frac{1}{2}U \left[1 + \sqrt{1 + 16t^2/U^2} \right] ,$$

$$\begin{aligned}\psi_4 = & -\sin\theta (| \uparrow, \downarrow \rangle + | \downarrow, \uparrow \rangle) \\ & + \cos\theta (| \uparrow\downarrow, \circ \rangle + | \circ, \uparrow\downarrow \rangle) ,\end{aligned}$$

$$\tan\theta = 4t / \left[U + \sqrt{U^2 + 16t^2} \right] .$$

Solving the Hubbard Model: 2-Site

ψ_1 is singlet, ψ_2 is triplet and the energy gap is

$$\begin{aligned}\Delta &= E_2 - E_1 = \frac{1}{2}U \left[\sqrt{1 + 16t^2/U^2} - 1 \right] \\ &\rightarrow \frac{4t^2}{U}, \quad \text{as } U \gg t \quad \theta \rightarrow 0.\end{aligned}$$

This leads to the Heisenberg model

$$H = J\mathbf{S}_1 \cdot \mathbf{S}_2 = \frac{J}{2} \left[\mathbf{S}^2 - \mathbf{S}_1^2 - \mathbf{S}_2^2 \right] = \begin{cases} \frac{1}{4}J \text{ triplet} \\ -\frac{3}{4}J \text{ singlet} \end{cases}$$

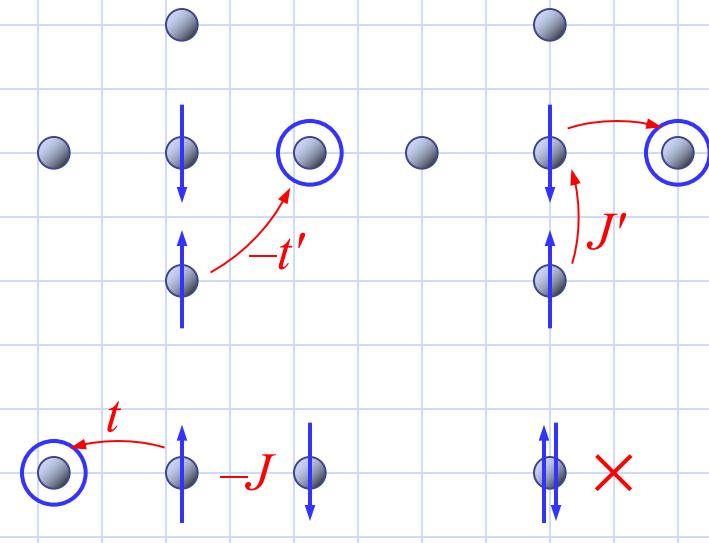
with $J = 4t^2/U$.

Strong Coupling Limit ($U \gg t$)

- Eliminate Double Occupied States
- 2nd order Degenerate Perturbation Theory (Schrieffer-Wolff Transformation)

$$H_{SC} = H_{t-J} + -t' \sum_{\langle i,j,k \rangle, \sigma} (c_{i,\sigma}^\dagger n_{j,-\sigma} c_{k,\sigma} + H.c) \\ + J' \sum_{\langle i,j,k \rangle, \sigma} (c_{i,\sigma}^\dagger c_{j,-\sigma}^\dagger c_{j,\sigma} c_{k,-\sigma} + H.c)$$

$$H_{t-J} = -t \sum_{\langle i,j \rangle, \sigma} (c_{i,\sigma}^\dagger c_{j,\sigma} + H.c) \\ + J \underbrace{\sum_{\langle i,j \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} n_i n_j)}_{\text{Heisenberg Model}}$$



- 1/2-Filled Band: AF Heisenberg Model
- $J = 4t^2/U, t' = J' = t^2/U$ (taken as free parameters)