



UCDAVIS



# Introduction to the Hubbard Hamiltonian

1. Creation and Destruction Operators
2. The Hubbard Hamiltonian
3. Non-interacting limit: “band structure” of the Hubbard Hamiltonian
4. Strong coupling limit: Mott gap and moment formation
5. Exact diagonalization: Mapping to Heisenberg model
6. Quick Overview of Related Analytic Treatments

Main goal: Insight into Hubbard Hamiltonian via solution in simple limits.

Find me any time to chat/ask questions about the book chapter, etc!

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## 1. Creation and Destruction Operators

Familiar  $a^\dagger, a$  for quantum harmonic oscillator:

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}} \hat{x} + i \sqrt{\frac{1}{2m\omega\hbar}} \hat{p} \quad \hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}} \hat{x} - i \sqrt{\frac{1}{2m\omega\hbar}} \hat{p}$$

$[\hat{p}, \hat{x}] = -i\hbar$  implies **commutation relations**,  $[\hat{a}, \hat{a}^\dagger] = 1$ .

Quantum Oscillator **Hamiltonian**:

$$\hat{H} = \frac{1}{2m} \hat{p}^2 + \frac{1}{2} m\omega^2 \hat{x}^2 = \hbar\omega \left( \hat{a}^\dagger \hat{a} + \frac{1}{2} \right) = \hbar\omega \left( \hat{n} + \frac{1}{2} \right)$$

with '**number operator**,'  $\hat{n} = \hat{a}^\dagger \hat{a}$ .

Ground state,  $|0\rangle$ :

$$\hat{a}|0\rangle = 0 \quad \hat{H}|0\rangle = \frac{\hbar\omega}{2} |0\rangle$$

Excited states,  $|n\rangle$ :

$$\hat{a}^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle \quad \hat{H}|n\rangle = \hbar\omega \left( n + \frac{1}{2} \right) |n\rangle$$

Finite temperature expectation value of quantum mechanical operator  $\hat{A}$ :

$$\langle \hat{A} \rangle = Z^{-1} \text{Tr}[\hat{A} e^{-\beta \hat{H}}]$$

For  $\hat{A} = \hat{n}$ , Bose-Einstein distribution function:

$$\langle \hat{n} \rangle = 1/(e^{\beta \hbar \omega} - 1).$$

$\hat{a}$  and  $\hat{a}^\dagger$ : ‘**boson**’ creation and destruction operators.

Henceforth, set  $\hbar = 1$  and  $k_B = 1$ .

Hubbard Hamiltonian: ‘**fermion**’ creation and destruction operators.

**Conceptual difference**: do not arise from position and momentum operators.

**Feynman Nobel Prize acceptance speech (development of meson theory)**:

*“I didn’t have the knowledge to understand the way these were defined in the conventional papers because they were expressed at that time in terms of creation and annihilation operators, and so on, which, I had not successfully learned. I remember that when someone had started to teach me about creation and annihilation operators, that this operator creates an electron, I said, ‘how do you create an electron? It disagrees with the conservation of charge’, and in that way, I blocked my mind from learning a very practical scheme of calculation”.*

Another different feature for the Hubbard Hamiltonian:

**Collection** of creation and destruction operators:

$\hat{c}_{\mathbf{j}\sigma}^\dagger$  ( $\hat{c}_{\mathbf{j}\sigma}$ ) create (destroy) electrons of spin  $\sigma$  on site  $\mathbf{j}$ .

States labeled by **multiple** occupation numbers:

$|n\rangle \rightarrow |n_{1\uparrow} n_{2\uparrow} n_{3\uparrow} \dots n_{1\downarrow} n_{2\downarrow} n_{3\downarrow} \dots\rangle$ .

Operators describe fermions: **Anticommutation** relations:  $\{\hat{A}, \hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A}$ .

$$\{\hat{c}_{\mathbf{j}\sigma}, \hat{c}_{\mathbf{l}\sigma'}^\dagger\} = \delta_{\mathbf{j},\mathbf{l}}\delta_{\sigma,\sigma'} \quad \{\hat{c}_{\mathbf{j}\sigma}^\dagger, \hat{c}_{\mathbf{l}\sigma'}^\dagger\} = 0 \quad \{\hat{c}_{\mathbf{j}\sigma}, \hat{c}_{\mathbf{l}\sigma'}\} = 0.$$

Like bosonic case,  $\hat{c}_{\mathbf{j}\sigma}^\dagger|0\rangle = |1\rangle$  creates electron from vacuum.

However,  $\hat{c}_{\mathbf{j}\sigma}^\dagger|1\rangle = \hat{c}_{\mathbf{j}\sigma}^\dagger\hat{c}_{\mathbf{j}\sigma}^\dagger|0\rangle = 0$ .

**Pauli principle!** Maximum occupation of a particular site with a given spin is 1.

Anticommutation  $\hat{c}_{j\sigma}^\dagger \hat{c}_{l\sigma}^\dagger = -\hat{c}_{l\sigma}^\dagger \hat{c}_{j\sigma}^\dagger$  ensures wave function **antisymmetry**.

**Convention** required for building states from vacuum:  $|\text{vac}\rangle = |00000\dots\rangle$ .

$|10100\dots\rangle = \hat{c}_1^\dagger \hat{c}_3^\dagger |\text{vac}\rangle$ ; and  $|10100\dots\rangle = \hat{c}_3^\dagger \hat{c}_1^\dagger |\text{vac}\rangle$  differ by sign.

Essential that convention chosen be followed consistently!

**Example:** Arises from **periodic boundary conditions**, electron moves site  $1 \leftrightarrow N$ .

$$\begin{aligned} \hat{c}_1^\dagger \hat{c}_N |\text{vac}\rangle &= \hat{c}_1^\dagger \hat{c}_N \hat{c}_3^\dagger \hat{c}_N^\dagger |\text{vac}\rangle \\ &= -\hat{c}_1^\dagger \hat{c}_3^\dagger \hat{c}_N \hat{c}_N^\dagger |\text{vac}\rangle = -\hat{c}_1^\dagger \hat{c}_3^\dagger (1 - \hat{c}_N^\dagger \hat{c}_N) |\text{vac}\rangle \\ &= -\hat{c}_1^\dagger \hat{c}_3^\dagger |\text{vac}\rangle = -|10100\dots000\rangle \end{aligned}$$

Rule: ‘jump over’ **odd** number of occupied sites (‘1’)  $\rightarrow$  **minus sign**.

If convention not followed carefully, things break, e.g. two noninteracting electrons will not have energy which is sum of single electron energies!

## 2. The Hubbard Hamiltonian

$$\hat{H} = -t \sum_{\langle \mathbf{ij} \rangle \sigma} (c_{\mathbf{i}\sigma}^\dagger c_{\mathbf{j}\sigma} + c_{\mathbf{j}\sigma}^\dagger c_{\mathbf{i}\sigma}) + U \sum_{\mathbf{i}} (n_{\mathbf{i}\uparrow} - \frac{1}{2})(n_{\mathbf{i}\downarrow} - \frac{1}{2}) - \mu \sum_{\mathbf{i}\sigma} (n_{\mathbf{i}\sigma} + n_{\mathbf{i}\sigma})$$

- $c_{\mathbf{i}\sigma}^\dagger$  ( $c_{\mathbf{i}\sigma}$ ) are fermion creation(destruction) operators, site  $\mathbf{i}$ , spin  $\sigma = \uparrow, \downarrow$ .
- Kinetic energy  $t$  describes hopping between near-neighbor sites  $\langle \mathbf{ij} \rangle$ .
- Chemical potential  $\mu$  controls filling.
- Describes qualitative “strong correlation” physics of many-electron materials

Transition metal monoxides, cuprate superconductors, ...

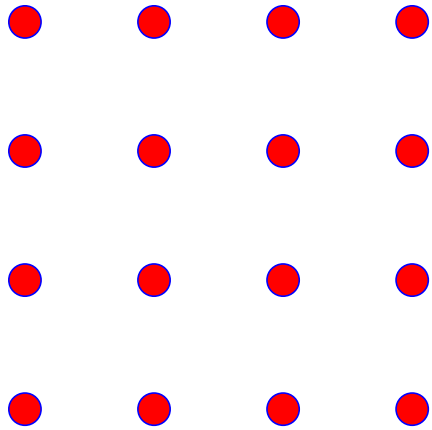
On-site repulsion  $U$  sufficiently large  $\rightarrow$  Mott Insulator

Exchange interaction  $J \propto t^2/U \rightarrow$  Antiferromagnetism

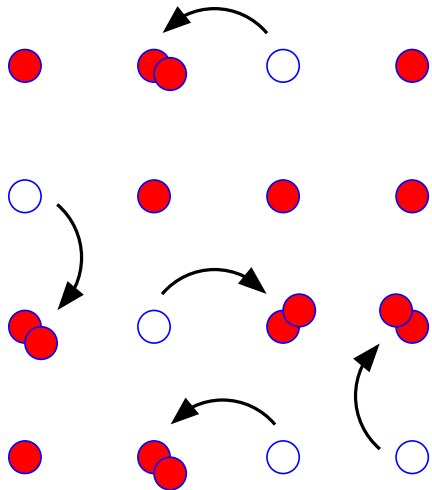
Stripes and other charge/spin inhomogeneities.

$d$ -wave superconductivity ???

## Mott Insulators and Antiferromagnetism: Qualitative Pictures

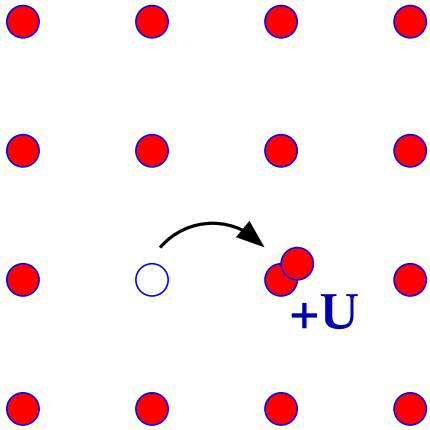


Consider a lattice of sites with  
“commensurate filling”:  
The **average** number of electrons  
is one per site.

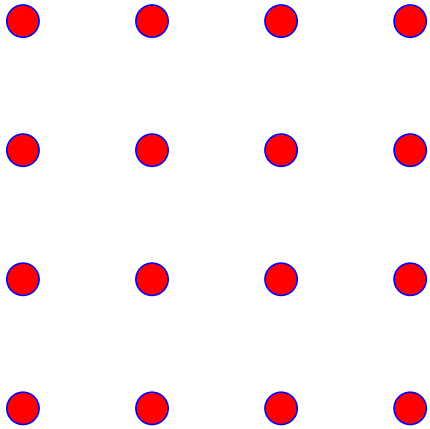


“quantum fluctuations” (kinetic energy  $t$ )  
and thermal fluctuations  $T$ , both favor  
electrons moving around lattice.

**Metal:** odd number (one) particle per cell/site.



But what if there were a large repulsive interaction  $U$  between electrons on the same site?



A **Mott Insulator** forms.  
Basic physics of parent compounds  
of cuprate superconductors!



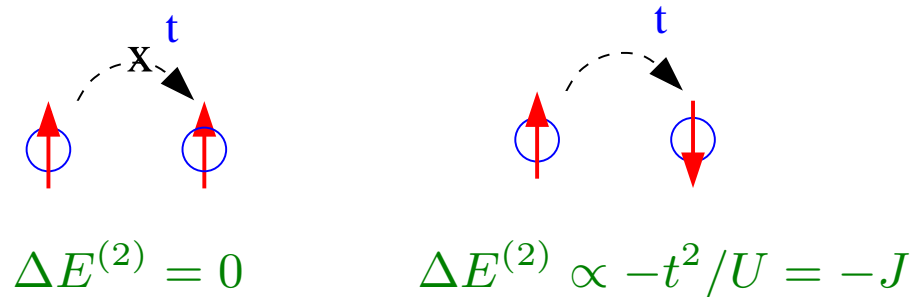
## Two ways to destroy Mott Insulator:

- \* Decrease  $U/t$ : By applying pressure (MnO)
- \* Shift  $\langle n \rangle \neq 1$ : Dope chemically (cuprate superconductors)

## What is optimal spin arrangement?

Hopping of neighboring **parallel** spins forbidden by Pauli.

**Antiparallel** arrangement lower in second order perturbation theory.



Mott insulating behavior and antiferromagnetism go hand-in-hand.  
Qualitative picture of cuprate physics **before doping**.

**Still do not fully understand why cuprates superconduct after doping.**

### 3. Non-interacting limit: “band structure” of the Hubbard Hamiltonian

Two alternate (but equivalent) solutions at  $U = 0$ .

One works in **real space**. The other in **momentum space**.

Start with the **real space** analysis: (useful in exact diagonalization approach later):

$\hat{H}$  commutes with the **total number operators**  $N_{\uparrow} = \sum_{\mathbf{j}} n_{\mathbf{j}\uparrow}$  and  $N_{\downarrow} = \sum_{\mathbf{j}} n_{\mathbf{j}\downarrow}$

Commutator of the kinetic energy on ‘link’ of the lattice with density at vertices:

$$[c_{i\sigma}^{\dagger} c_{j\sigma} + c_{j\sigma}^{\dagger} c_{i\sigma}, n_{i\sigma} + n_{j\sigma}] = 0$$

Handy identity:  $[AB, C] = A\{B, C\} - \{A, C\}B$ .

Hopping contains creation and annihilation operators in pairs.

Implication: eigenstates of  $\hat{H}$  come in **separate sectors** of total  $N_{\uparrow}$  and  $N_{\downarrow}$ .

Consider **single particle sector** where  $N_{\uparrow} = 1$  and  $N_{\downarrow} = 0$ .

Occupation number **basis**:  $|100000\dots\rangle, |010000\dots\rangle, |001000\dots\rangle, \dots$

Examine one-d linear chain.  $\hat{H}$  moves occupied site to the left or right:

$$\hat{H} |010000\dots\rangle = -\mu |010000\dots\rangle - t |100000\dots\rangle - t |001000\dots\rangle$$

Matrix for  $\hat{H}$ , use periodic boundary conditions (pbc):

$$H = \begin{pmatrix} -\mu & -t & 0 & 0 & \dots & 0 & -t \\ -t & -\mu & -t & 0 & \dots & 0 & 0 \\ 0 & -t & -\mu & -t & \dots & 0 & 0 \\ 0 & 0 & -t & -\mu & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ -t & 0 & 0 & 0 & \dots & -t & -\mu \end{pmatrix}$$

Mathematical identity: Eigenvalues of NxN tridiagonal matrix

$$\lambda_n = -\mu - 2t \cos k_n \quad k_n = 2\pi n/N \quad n = 1, 2, 3, \dots, N.$$

Proof: use *ansatz*  $v_l = e^{ikl}$  in eigenvalue equation

$$\begin{aligned} -\mu v_l - t v_{l-1} - t v_{l+1} &= \lambda v_l. \\ (-\mu - t e^{-ik} - t e^{+ik}) e^{ikl} &= \lambda e^{ikl}. \end{aligned}$$

Discretization of  $k$  arises from pbc,  $v_0 = v_N$  and  $v_{N+1} = v_1$ .

Eigenvalues of  $U = 0$  Hubbard Hamiltonian in one particle sector (1d chain):

$$\text{“Energy band” : } \quad \epsilon(k) = -2t \cos k$$

Eigenvectors  $(\vec{v}_k)_l = e^{ikl}$  are Bloch states.

**Two particle sector:**  $N_\uparrow = 2$  and  $N_\downarrow = 0$ .

$N(N - 1)/2$  occupation number basis states:

$$|110000\dots\rangle, |101000\dots\rangle, |100100\dots\rangle, \dots$$

Same construction as  $N_\uparrow = 1$ : Act with  $\hat{H}$  on each state. Get the **matrix** for  $\hat{H}$ .

Diagonalizing yields  $N(N - 1)/2$  eigenvalues and eigenvectors.

Eigenvalues are sums of pairs of the eigenvalues of  $N_\uparrow = 1$  matrix

with the **Pauli Principle** restriction (choose distinct eigenvalues).

Similar result for all sectors  $N_\uparrow = 3, 4, 5, \dots$

**Interactions turn the Hubbard Hamiltonian into a *many body problem*.**

Second, treatment of  $U = 0$  limit ( $d = 1$ ). **Canonical transformation:**

$$c_{k\sigma}^\dagger = \frac{1}{\sqrt{N}} \sum_l e^{ikl} c_{l\sigma}^\dagger. \quad c_{l\sigma}^\dagger = \frac{1}{\sqrt{N}} \sum_k e^{-ikl} c_{k\sigma}^\dagger.$$

Momentum  $k$  discretized: same number of  $c_{k\sigma}^\dagger$  as  $c_{l\sigma}^\dagger$ .

Inverse relation follows from **orthogonality identities:**

$$\frac{1}{N} \sum_l e^{i(k-p)l} = \delta_{k,p} \quad \frac{1}{N} \sum_k e^{ik(l-j)} = \delta_{l,j}$$

These are discrete analog of  $\int dk e^{ikx} = 2\pi\delta(x)$ .

**Anticommutation relations preserved** (suppress spin indices):

$$\begin{aligned} \{c_k, c_p^\dagger\} &= \left\{ \frac{1}{\sqrt{N}} \sum_l e^{-ikl} c_l, \frac{1}{\sqrt{N}} \sum_m e^{+ipm} c_m^\dagger \right\} \\ &= \frac{1}{N} \sum_{l,m} e^{-ikl} e^{+ipm} \{c_l, c_m^\dagger\} \\ &= \frac{1}{N} \sum_{l,m} e^{-ikl} e^{+ipm} \delta_{l,m} = \sum_l e^{+i(p-k)m} \delta_{l,m} = \delta_{k,p} \end{aligned}$$

Transform  $d = 1$  noninteracting **Hubbard Hamiltonian** to momentum space:

$$\begin{aligned}
 \hat{H} &= -t \sum_l (c_{l+1}^\dagger c_l + c_l^\dagger c_{l+1}) \\
 &= -t \sum_l \frac{1}{N} \sum_k \sum_p (e^{ik(l+1)} e^{-ip l} + e^{ik l} e^{-ip(l+1)}) c_k^\dagger c_p \\
 &= -t \sum_k \sum_p \frac{1}{N} \sum_l e^{il(k-p)} (e^{ik} + e^{-ip}) c_k^\dagger c_p \\
 &= -t \sum_k \sum_p \delta_{k,p} (e^{ik} + e^{-ip}) c_k^\dagger c_p \\
 &= -t \sum_k (e^{ik} + e^{-ik}) c_k^\dagger c_k \\
 \hat{H} &= \sum_k \epsilon_k c_k^\dagger c_k = \sum_k \epsilon_k n_k
 \end{aligned}$$

Reproduce energy band  $\epsilon_k = -2t \cos k$ .

$\hat{H}$  resembles quantum oscillator.

**Sum of independent (mutually commuting) number operators.**

Evident that single particle levels  $\epsilon_k$  give solution for all particle sectors.

Once  $\epsilon_{\mathbf{k}}$  known, can compute statistical mechanics properties:

Partition function, density, internal energy, free energy, and entropy of the noninteracting **Hubbard Hamiltonian**:

$$\begin{aligned} Z &= \text{Tr} \left[ e^{-\beta \hat{H}} \right] = \prod_{\mathbf{k}} \sum_{n_{\mathbf{k}}=0,1} e^{-\beta(n_{\mathbf{k}}-\mu)} = \prod_{\mathbf{k}} (1 + e^{-\beta(\epsilon_{\mathbf{k}}-\mu)}) \\ \rho &= Z^{-1} \text{Tr} \left[ \sum_{\mathbf{k}} n_{\mathbf{k}} e^{-\beta \hat{H}} \right] = \sum_{\mathbf{k}} (1 + e^{-\beta(\epsilon_{\mathbf{k}}-\mu)})^{-1} = \sum_{\mathbf{k}} f_{\mathbf{k}} \\ E &= Z^{-1} \text{Tr} \left[ \hat{H} e^{-\beta \hat{H}} \right] = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} (1 + e^{-\beta(\epsilon_{\mathbf{k}}-\mu)})^{-1} = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} f_{\mathbf{k}} \\ S &= \beta (E - F) = \beta E - \ln Z \end{aligned}$$

with usual Fermi function  $f_{\mathbf{k}} = (1 + e^{-\beta(\epsilon_{\mathbf{k}}-\mu)})^{-1}$ .

Having computed  $\epsilon_{\mathbf{k}}$ , also valuable to obtain the **density of states** (DOS),

$$N(E) = \frac{1}{N} \sum_{\mathbf{k}} \delta(E - \epsilon_{\mathbf{k}}) \rightarrow (2\pi)^{-d} \int d\mathbf{k} \delta(E - \epsilon_{\mathbf{k}}).$$

DOS counts the number of energy levels having a particular value  $E$ .

$d = 1$  chain with  $\epsilon_k = -2t \cos k$  has  $N(E) = 1 / (\pi \sqrt{4t^2 - E^2})$ .

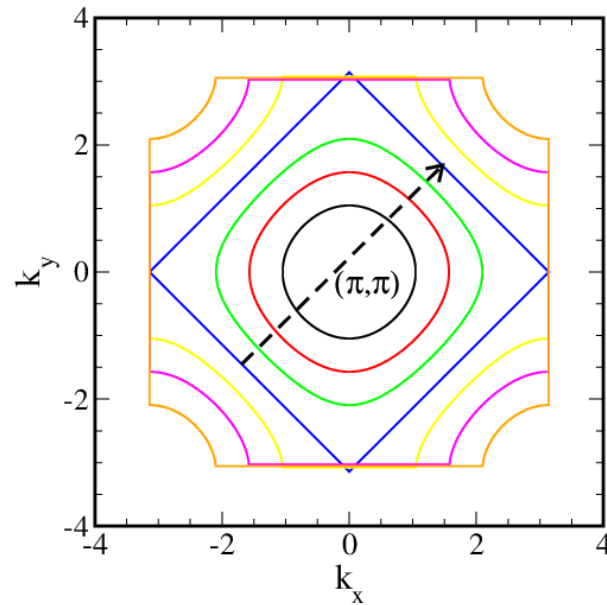
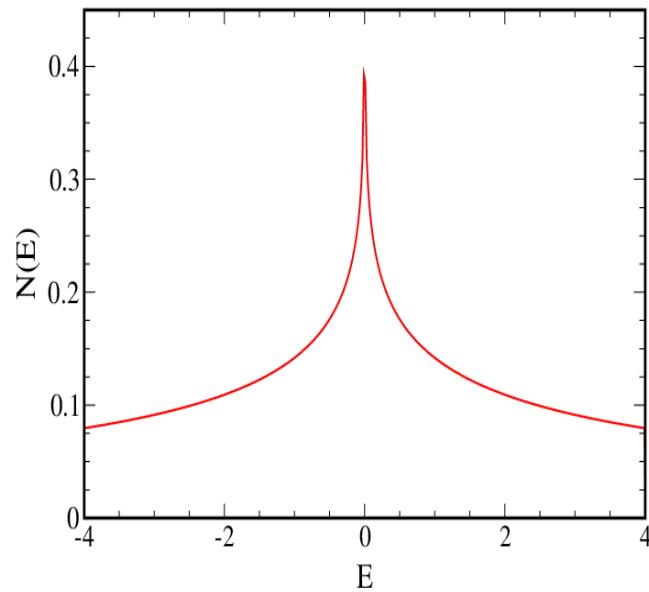
Informative to consider further examples of noninteracting **band structure**.

Square lattice is generalization of  $d = 1$  chain,

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

DOS of square lattice has a **van Hove singularity** at  $E_F = 0$  (half-filling).

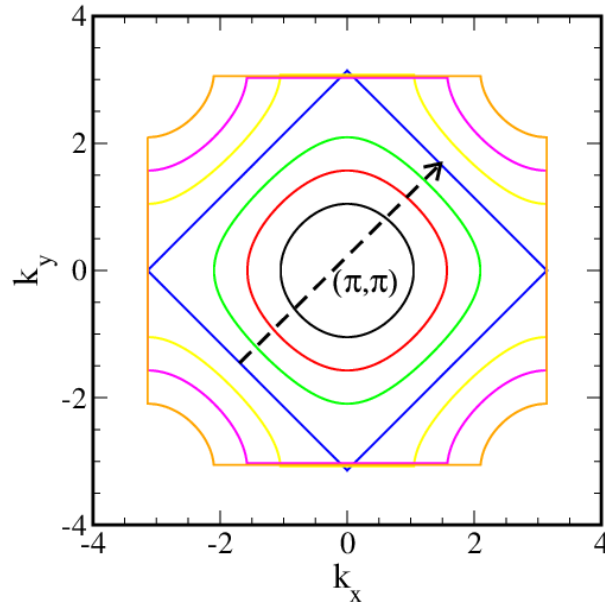
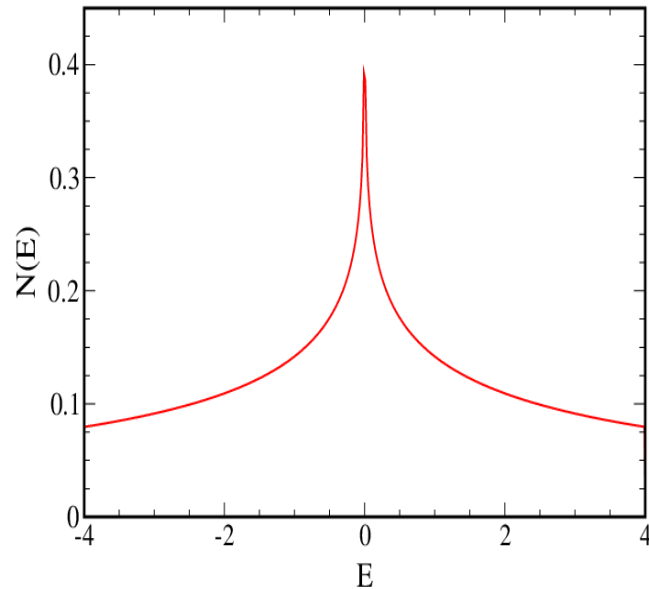
**Fermi surface** (contours of constant  $\epsilon_{\mathbf{k}}$ ) evolves from circles around  $(k_x, k_y) = (0, 0)$  at low filling, to a rotated square at half-filling  $\rho = 1$ .





Cuprate superconductors: copper atoms of  $\text{CuO}_2$  sheets reside on a square lattice.

Early theories: DOS singularity enhances  $T_c \sim \omega e^{-1/VN(E_F)}$  (BCS formula).



FS of square lattice also has unique feature at half-filling: **perfect nesting**.

Momentum  $\mathbf{k} = (\pi, \pi)$  maps large segments of the FS onto itself.

Suggests  $\mathbf{k} = (\pi, \pi)$  might play a crucial role. Indeed: **antiferromagnetic order**.

Another example: (d=1) Hubbard Hamiltonian with **staggered potential**,

$$\hat{H} = -t \sum_l (c_{l+1}^\dagger c_l + c_l^\dagger c_{l+1}) + \Delta \sum_l (-1)^l c_l^\dagger c_l$$

Write  $(-1)^l = e^{il\pi}$  and go to momentum space.

$$\Delta \sum_l (-1)^l c_l^\dagger c_l = \Delta \frac{1}{N} \sum_l e^{i\pi l} \sum_k e^{-ikl} c_k^\dagger \sum_p e^{+ipl} c_p = \Delta \sum_k c_k^\dagger c_{k+\pi}$$

$\hat{H}$  not fully diagonalized: **momenta  $k$  and  $k + \pi$  mix**.

$$H = \sum_k \begin{pmatrix} c_k^\dagger & c_{k+\pi}^\dagger \end{pmatrix} \begin{pmatrix} -2t \cos k & \Delta \\ \Delta & -2t \cos(k + \pi) \end{pmatrix} \begin{pmatrix} c_k \\ c_{k+\pi} \end{pmatrix}$$

$k$  sum is over the reduced Brillouin zone  $-\pi/2 < k < \pi/2$ .

Diagonalization of 2x2 matrix yields **two bands**  $E_k = \pm \sqrt{(-2t \cos k)^2 + \Delta^2}$ .

**Band gap  $2\Delta$**  opens at reduced Brillouin zone boundaries  $k = \pm\pi/2$ .

Analysis of energy bands in staggered potential identical mathematically to study of antiferromagnetism in mean field treatment of  $U \neq 0$  Hubbard Hamiltonian.

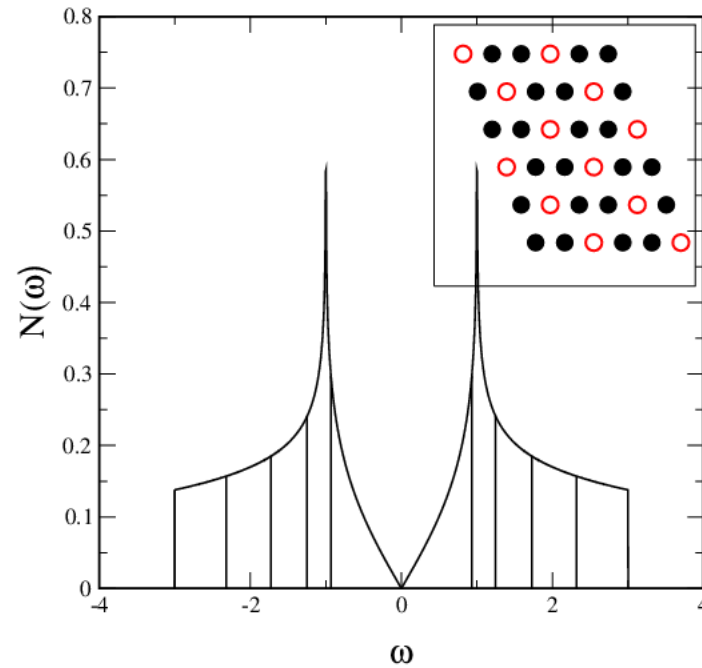
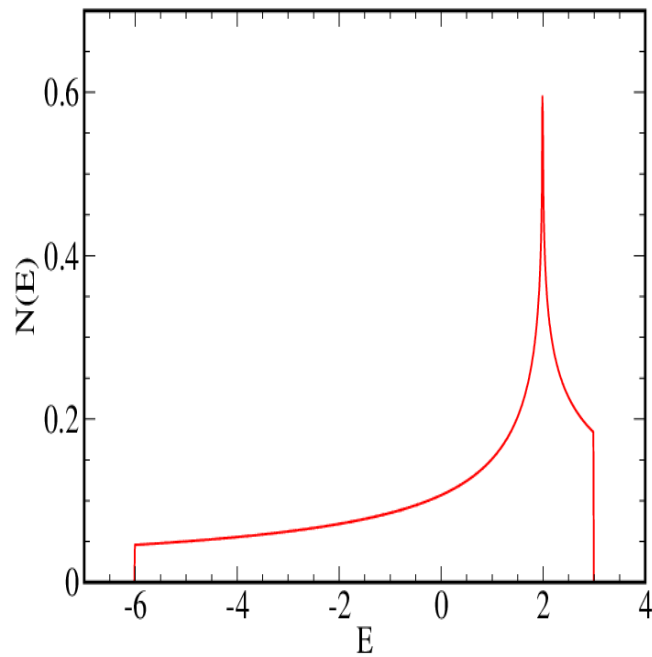
Band gap  $\rightarrow$  **Slater gap** arising in antiferromagnets below **Néel transition**.

DOS of the  $U = 0$  **triangular lattice** Hubbard Hamiltonian (Left).

The DOS of the  $U = 0$  **honeycomb lattice** Hubbard Hamiltonian (Right).

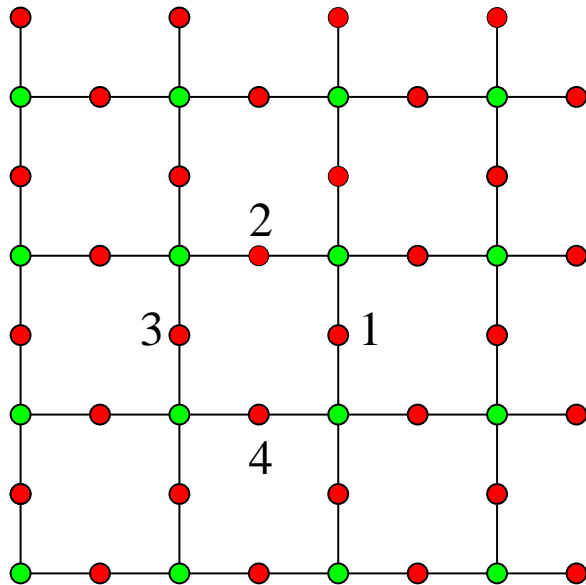
Honeycomb lattice notable for its **Dirac points** with  $\epsilon_k \sim k$  and

**linearly vanishing DOS** at half-filling.



Final example: 'Lieb lattice'.

More refined picture of the  $\text{CuO}_2$  planes of cuprate superconductors.



Topologically localized states

$$|\psi\rangle = (c_1^\dagger - c_2^\dagger + c_3^\dagger - c_4^\dagger) |\text{vac}\rangle$$

$$\hat{K}|\psi\rangle = 0$$

Same construction on any equivalent set of four sites on the lattice.

Degenerate set of states all with the same energy  $E = 0$ .

Form linear combinations: momentum states have flat energy band  $\epsilon_{\mathbf{k}} = 0$ .

Lieb has shown ferromagnetic order in the presence of such flat bands for  $U \neq 0$ .

Flat bands also arise in Kagome lattice.

## 4. Strong coupling limit: Mott gap and moment formation

If  $t = 0$ ,  $[\hat{H}, n_{\mathbf{j}\sigma}] = 0$  for each  $\mathbf{j}$ ,

Number operators also commute with each other:  $[\hat{n}_{\mathbf{i}\sigma'}, n_{\mathbf{j}\sigma}] = 0$ .

Consider terms in  $\hat{H} = U \sum_{\mathbf{i}} (n_{\mathbf{i}\uparrow} - \frac{1}{2})(n_{\mathbf{i}\downarrow} - \frac{1}{2})$  individually (single sites).

Four occupation number states:  $|0\rangle$   $|\uparrow\rangle$   $|\downarrow\rangle$   $|\uparrow\downarrow\rangle$ .

Each is already an eigenstate of  $\hat{H} = U(n_{\uparrow} - \frac{1}{2})(n_{\downarrow} - \frac{1}{2})$ .

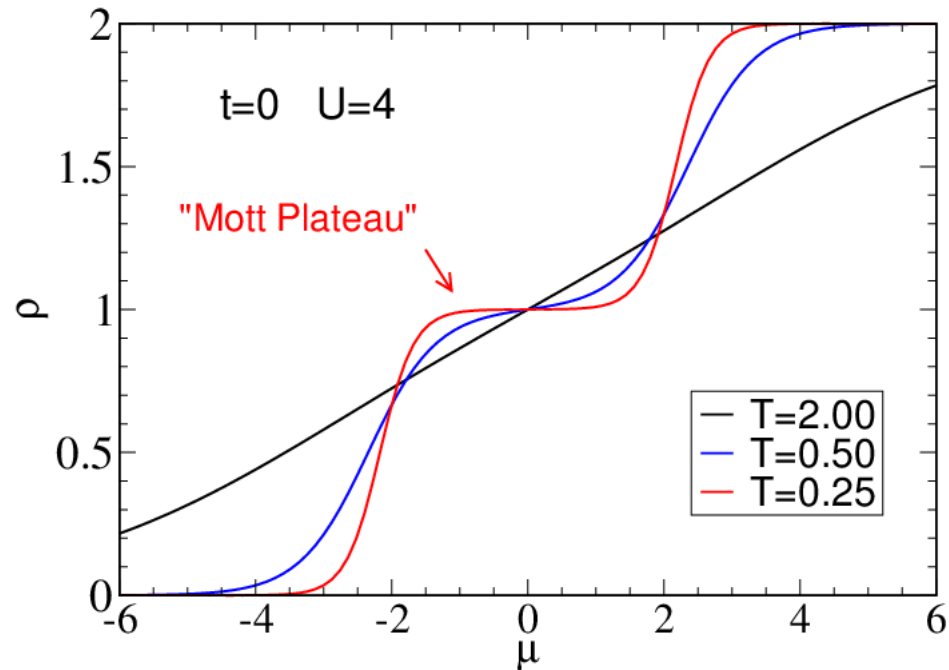
Eigenvalues:  $U/4$   $-U/4 - \mu$   $-U/4 - \mu$   $U/4 - 2\mu$ .

Partition function and occupation,

$$Z = \text{Tr} [e^{-\beta\hat{H}}] = e^{-\beta U/4} + 2e^{-\beta(-U/4-\mu)} + e^{-\beta(U/4-2\mu)}$$

$$\rho = Z^{-1} \text{Tr} [(n_{\uparrow} + n_{\downarrow}) e^{-\beta\hat{H}}] = Z^{-1} (2e^{-\beta(-U/4-\mu)} + 2e^{-\beta(U/4-2\mu)})$$

Note **particle-hole symmetry**:  $\rho = 1$  at  $\mu = 0$  for all  $\beta U$ .



As the temperature  $T$  decreases, a “Mott Plateau” develops:  
 Increasing  $\mu$  initially adds fermions, but  $\rho$  gets frozen at  $\rho = 1$ .  
 Chemical potential must jump by  $\Delta\mu = U$  to add a second fermion.  
 The **compressibility**  $\kappa = \partial\rho/\partial\mu = 0$  in the Mott gap.

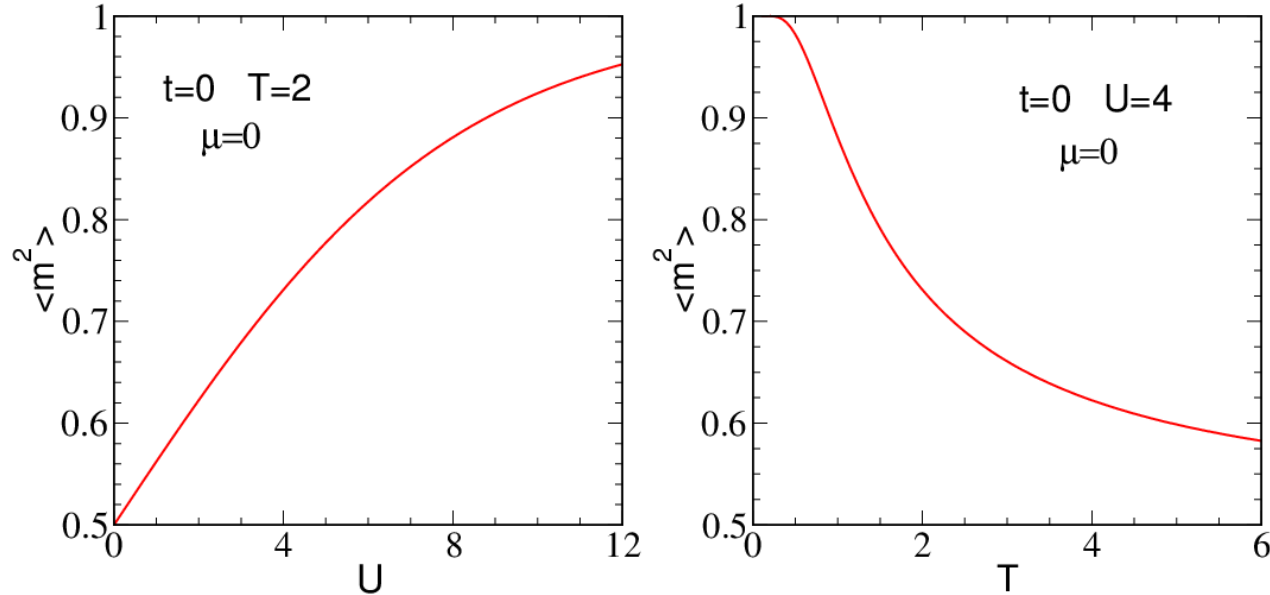
## 'Local moment'

$$\langle m^2 \rangle = \langle (n_\uparrow - n_\downarrow)^2 \rangle = \langle n_\uparrow + n_\downarrow \rangle - 2\langle n_\uparrow n_\downarrow \rangle = \rho - 2D$$

$D = \langle n_\uparrow n_\downarrow \rangle$  is the 'double occupancy'.

$\langle m^2 \rangle = 0$  if site is empty ( $|0\rangle$ ) or doubly occupied ( $|\uparrow\downarrow\rangle$ ).

$\langle m^2 \rangle = 1$  if the site has a single fermion ( $|\uparrow\rangle$  or  $|\downarrow\rangle$ ).



$\mu = 0$  (half-filling): Local moments develop as  $T$  is reduced or  $U$  is increased.

## 5. Exact diagonalization: Mapping to Heisenberg model

Strong coupling (single site): insight into the role of  $U$  in

- Moment formation.
- Development of Mott plateau.

Need  $t \neq 0$  for interplay of kinetic and potential energy

- Formation of **intersite magnetic correlations**.

Examine Hubbard Hamiltonian HH on two spatial sites.

Simplest non-trivial example of powerful **exact diagonalization** method.

Occupation number basis for two sites:  $|n_{1\uparrow} n_{1\downarrow} n_{2\uparrow} n_{2\downarrow}\rangle$

$t \neq 0$  gives fermion number (“quantum”) fluctuations on **individual** sites.

$$[\hat{H}, n_{1\uparrow}] \neq 0 \quad [\hat{H}, n_{1\downarrow}] \neq 0 \quad [\hat{H}, n_{2\uparrow}] \neq 0 \quad [\hat{H}, n_{2\downarrow}] \neq 0$$

$\hat{H}$  still commutes with **total** up and down occupation:

$$[\hat{H}, n_{1\uparrow} + n_{2\uparrow}] = [\hat{H}, n_{1\downarrow} + n_{2\downarrow}] = 0$$



$2^4 = 16$  dimensional Hilbert space divides into **nine sectors**.

$$(n_{1\uparrow} + n_{2\uparrow}, n_{1\downarrow} + n_{2\downarrow}) = (0, 0), (1, 0), (2, 0), (0, 1), (1, 1), (2, 1), (0, 2), (1, 2), (2, 2)$$

Dimensions 1, 2, 1, 2, 4, 2, 1, 2, 1 respectively.

$\hat{H}$  is block diagonal.

Sectors of dimension 1 immediately identify four eigenstates:

Empty lattice, (0,0) sector:  $|n_{1\uparrow} n_{1\downarrow} n_{2\uparrow} n_{2\downarrow}\rangle = |0000\rangle$

Packed lattice (2,2) sector:  $|n_{1\uparrow} n_{1\downarrow} n_{2\uparrow} n_{2\downarrow}\rangle = |1111\rangle$

Two same spin electrons (2,0), (0,2) sectors:  $|n_{1\uparrow} n_{1\downarrow} n_{2\uparrow} n_{2\downarrow}\rangle = |1010\rangle, |0101\rangle$

All have zero kinetic energy. **Pauli Principle** blocks hopping.

Denote by # a site which is doubly occupied, and by \* a site that is empty.

$$|\uparrow\uparrow\rangle, |\downarrow\downarrow\rangle \quad (2, 0) \text{ and } (0, 2) \text{ energies are } -U/2 \text{ (remember these).}$$

$$|**\rangle, |##\rangle \quad (0, 0) \text{ and } (2, 2) \text{ energies are } +U/2.$$

As seen at  $t = 0$ :  $U$  favors local moment on each site.

Four sectors (1, 0), (0, 1), (2, 1), (1, 2) of dimension two have eigenenergies  $\pm t$ .

Single fermion can hop between sites.

(1, 1) sector has dimension four.

Act with  $\hat{H}$  on four states  $|\uparrow \downarrow\rangle, |\downarrow \uparrow\rangle, |\# * \rangle, |* \# \rangle$ . Get matrix

$$\hat{H} = \begin{pmatrix} -U/2 & 0 & -t & -t \\ 0 & -U/2 & -t & -t \\ -t & -t & U/2 & 0 \\ -t & -t & 0 & U/2 \end{pmatrix}$$

Eigenvalues are  $-U/2, U/2, \pm\sqrt{4t^2 + U^2/4}$ .

We have the complete spectrum of the two site Hubbard Hamiltonian.

In contrast to  $U = 0$ , **cannot** infer all eigenenergies from single particle sector.

Low temperature properties determined by the lowest energy eigenstates.

Energies  $-U/2$  (threefold degenerate), and  $-\sqrt{4t^2 + U^2/4}$ .

$U \gg t$ : expand  $-\sqrt{4t^2 + U^2/4} \approx -U/2 - 4t^2/U$

Mapping to the spin-1/2 Heisenberg Hamiltonian when  $U \gg t$ .

Two site, spin-1/2 Heisenberg Hamiltonian

$$\hat{H} = J \vec{S}_1 \cdot \vec{S}_2 = J/2 \left( (\vec{S}_1 + \vec{S}_2)^2 - \vec{S}_1^2 - \vec{S}_2^2 \right),$$

Spin-1/2: each site can have  $S_z = \pm 1/2$ .

Adding two spin-1/2: spin-0 ('singlet') or spin-1 ('triplet').

Square of total spin:  $(\vec{S}_1 + \vec{S}_2)^2 = 0, 2$ .  $\vec{S}_1^2 = \vec{S}_2^2 = 3/4$ .

Solution of two site Heisenberg model:

$$J \vec{S}_1 \cdot \vec{S}_2 = J (0 - 3/4 - 3/4) = -3J/4 \text{ (singlet)}$$

$$J \vec{S}_1 \cdot \vec{S}_2 = J (2 - 3/4 - 3/4) = +J/4 \text{ (triplet)}$$

Heisenberg Spectrum: one state of energy  $-3J/4$ ; three states of energy  $+J/4$ .

In large  $U$  limit, two site Hubbard Hamiltonian has same structure:

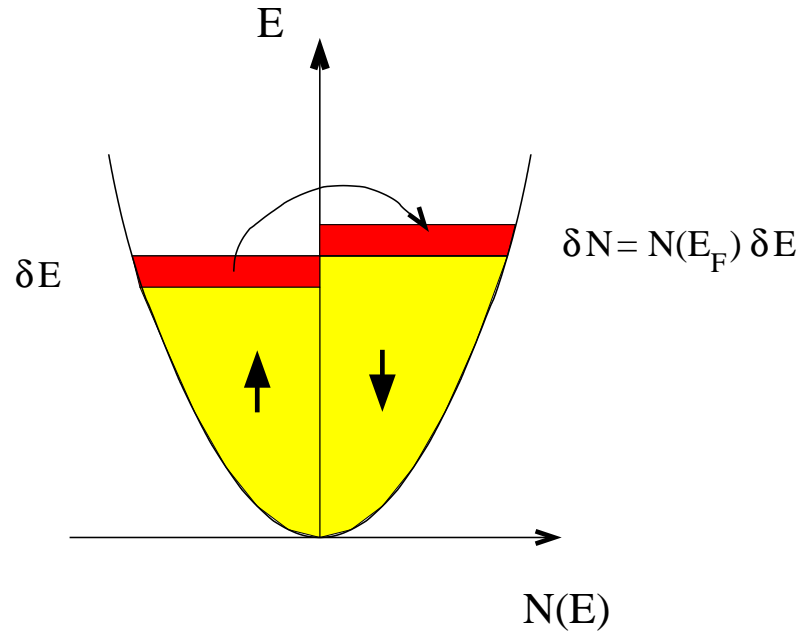
One state of energy  $-U/2 - 4t^2/U$ . Three states of energy  $-U/2$ .

Hubbard and Heisenberg eigenspectra are identical. Exchange energy  $J = 4t^2/U$ .

Same  $J$  as previously in second order perturbation theory picture.)

With computer, exact diagonalization can be extended to larger numbers of sites.

## 6. Quick Overview of Related Analytic Treatments



“Stoner” Picture of Magnetic Order

Density of states

$$N(E_F) = \delta N / \delta E \propto 1/t$$

Interaction energy lowered by polarizing the spins:

$$\delta PE = U(N + \delta N)(N - \delta N) - UN^2 = -U(\delta N)^2 = -UN(E_F) \delta N \delta E$$

Kinetic energy raised by polarizing the spins:

$$\delta KE = +\delta N \delta E$$

Total Energy change:

$$\delta E = \delta KE + \delta PE = [1 - UN(E_F)] \delta N \delta E$$

**Stoner Criterion:**  $UN(E_F) > 1$      $\delta E < 0 \rightarrow$  ferromagnetism!

**Mean-field theory (MFT)**; Replace quartic interaction terms by quadratic.

$$Un_{i\uparrow}n_{i\downarrow} \rightarrow U [n_{i\uparrow}\langle n_{i\downarrow} \rangle + \langle n_{i\uparrow} \rangle n_{i\downarrow} - \langle n_{i\uparrow} \rangle \langle n_{i\downarrow} \rangle]$$

Because **quadratic** the same  $U = 0$  ‘band structure’ techniques work.

**Antiferromagnetic order** in MFT: *ansatz*  $\langle n_{i\uparrow} \rangle = -\langle n_{i\downarrow} \rangle = (-1)^i m_{\text{af}}$ .

Therefore, MFT treatment identical to ‘**staggered potential**’ analysis!

Related to **Random Phase Approximation** for magnetic susceptibility  $\chi$ ,

$$\chi(q, \omega) = \frac{\chi_0(q, \omega)}{1 - U\chi_0(q, \omega)} \quad \chi_0(q, \omega) = \sum_p \frac{f(\epsilon_k) - f(\epsilon_{k+q})}{\omega - (\epsilon_k - \epsilon_{k+q})}$$

Fermi function:  $f(\epsilon_k) = [e^{\beta(\epsilon_k - \mu)} + 1]^{-1}$ .

Interacting  $\chi$  is increased ( $1 - U\chi_0 < 1$ ): **Stoner Enhancement**.

Generalization of Stoner criterion ( $1 - UN(E_F) < 1$ ) to  $q \neq 0$ .

Ordering wavevector  $q$  determined by which  $\chi(q, \omega = 0)$  reaches  $1/U$  first.

**MFT very useful, but important failure:**

Predicts  $T_{\text{Neel}} \propto U$  at large  $U$ .

Instead,  $T_{\text{Neel}} \propto J = t^2/U$  at large  $U$ .

A graduate student enjoys the Stoner Enhancement.



(Courtesy of Dan Arovas.)