

# Introduction to the Hubbard Model

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Prelude: 3d transition metals and their compounds

What makes the 3d transition metals special: small radius of their 3d shell



Taken from: D. van der Marel and G. A. Sawatzky, Phys. Rev. B 37, 10674 (1988).

The small spatial extent of the 3d shell enhances the Coulomb repulsion between electrons strongly



Up to 10eV increase in energy!

To study the motion of conduction electrons under the influence of this strong Coulomb repulsion Hubbard, Gutzwiller and Kanamori more or less simultaneously introduced a simplified model, nowadays known as the Hubbard model

After the discovery of the copper oxide superconductors and after Zhang and Rice showed that these materials can be described by the 2D Hubbard model there was renewed interest in the Hubbard model

The Hubbard model is highly oversimplified:

- All atoms besides the transition metal atoms are ignored
- The five-fold degeneracy of the 3d orbital is neglected one s-like orbital/site

$$\begin{array}{cccc} & & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ &$$



An important additional parameter in this model is the density of electrons

We call N the number of sites,  $N_e = N_{\uparrow} + N_{\downarrow}$  the number of electrons - densities are denotes by n:  $n_{\uparrow} = N_{\uparrow}/N$ For copper oxide supercondutors the important range of densities is  $1 \ge n_e \ge 0.7$  and  $U/t \approx 10$  $n_e = 1$  means  $n_{\uparrow} = n_{\downarrow} = \frac{1}{2}$  - i.e. a metal with a half-filled band for noninteracting electrons In contrast to this the cuprates are insulators for  $n_e = 1$  - i.e. Mott insulators The imaginary time Green's function is (with  $c(\tau) = e^{\tau(H-\mu N)} c e^{-\tau(H-\mu N)}$ )

$$G_{\sigma}(\boldsymbol{k},\tau) = -\langle T c_{\boldsymbol{k},\sigma}(\tau) c_{\boldsymbol{k},\sigma}^{\dagger} \rangle_{th} = -\Theta(\tau) \langle c_{\boldsymbol{k},\sigma}(\tau) c_{\boldsymbol{k},\sigma}^{\dagger} \rangle_{th} + \Theta(-\tau) \langle c_{\boldsymbol{k},\sigma}^{\dagger} c_{\boldsymbol{k},\sigma}(\tau) \rangle_{th}$$

 $G(\tau)$  has the Fourier transform (with  $i\omega_{\nu}$ : (Fermionic) Matsubara frequencies)

$$G(\tau) = \frac{1}{\beta} \sum_{\nu = -\infty}^{\infty} e^{-i\omega_{\nu}\tau} G(i\omega_{\nu})$$
$$G(i\omega_{\nu}) = \int_{0}^{\beta} d\tau \ e^{i\omega_{\nu}\tau} G(\tau)$$
$$\omega_{\nu} = \frac{(2\nu + 1)\pi}{\beta}$$

The Fourier coefficient  $G_{\sigma}(\mathbf{k}, i\omega_{\nu})$  is given by the Lehmann representation (where  $H|j\rangle = E_j|j\rangle$ ):

$$G_{\sigma}(\boldsymbol{k}, i\omega_{\nu}) = \frac{1}{Z} \sum_{i,j} \frac{e^{-\beta(E_{i}-\mu N_{i})} + e^{-\beta(E_{j}-\mu N_{j})}}{i\omega_{\nu} + \mu - (E_{j} - E_{i})} |\langle i| c_{\boldsymbol{k},\sigma} |j\rangle|^{2}$$

Lehmann representation of  $G_{\sigma}(\mathbf{k}, i\omega_{\nu})$ :

$$G_{\sigma}(\boldsymbol{k}, i\omega_{\nu}) = \frac{1}{Z} \sum_{i,j} \frac{e^{-\beta(E_{i}-\mu N_{i})} + e^{-\beta(E_{j}-\mu N_{j})}}{i\omega_{\nu} + \mu - (E_{j}-E_{i})} |\langle i| c_{\boldsymbol{k},\sigma} |j\rangle|^{2}$$

 $G_{\sigma}(\mathbf{k}, i\omega_{\nu})$  can be analytically continued -  $G_{\sigma}(\mathbf{k}, \omega + i0^{+})$  is (the Fourier transform of) the retarded real-time Green's function - this gives the combined photoemission and inverse photoemission spectrum of the system

$$A(\mathbf{k},\omega) = -\frac{1}{\pi} \lim_{\epsilon \to 0} \mathcal{I} G_{\sigma}(\mathbf{k},\omega+i\epsilon) = Z_{\mathbf{k}}^{(-)} \delta(\omega-E_{\mathbf{k}}^{(-)}) + Z_{\mathbf{k}}^{(+)} \delta(\omega-E_{\mathbf{k}}^{(+)})$$

The poles of  $G_{\sigma}(\mathbf{k},\omega)$  give the ionization and electron affinity energies - i.e. the quasiparticle energies

The self-energy is defined by the Dyson equation

$$(\omega + \mu - \epsilon_{\mathbf{k}} - \Sigma(\mathbf{k}, \omega)) G(\mathbf{k}, \omega) = 1.$$

Lehmann representation of  $G(\mathbf{k},\omega)$  (*n* runs over pairs (*i*, *j*)):

$$G(\boldsymbol{k},\omega) = \frac{1}{Z} \sum_{i,j} \frac{e^{-\beta(E_i - \mu N_i)} + e^{-\beta(E_j - \mu N_j)}}{\omega + \mu - (E_j - E_i)} |\langle i| c_{\boldsymbol{k},\sigma} |j\rangle|^2 = \sum_n \frac{\alpha_n}{\omega - \omega_n}$$

with  $\alpha_n$ ,  $\omega_n$  real  $\Rightarrow$  For real  $\omega$   $G(\omega)$  looks like this:





Near a zero  $\zeta_i$  :

$$G(\omega) \approx -\beta_i (\omega - \zeta_i)$$

The Dyson equation:

$$G^{-1}(\omega) = \omega + \mu - \epsilon_{\mathbf{k}} - \Sigma(\omega)$$
  

$$\Rightarrow \Sigma(\omega) = -G^{-1}(\omega) + \omega + \mu - \epsilon_{\mathbf{k}} = \frac{1/\beta_i}{\omega - \zeta_i} + \dots$$

 $\Sigma(\omega)$  has simple poles at the zeros of the Green's function,  $\zeta_i$ 

Luttinger has shown that  $\Sigma(\omega)$  can be written as (with  $\sigma_i = 1/\beta_i > 0$ ,  $V_{HF}$ : Hartree-Fock potential)

$$\Sigma(\omega) = V_{HF} + \sum_{i} \frac{\sigma_i}{\omega - \zeta_i}$$

• We consider the Hubbard model on a dimer - i.e. a two-atom system with atoms  $1 \mbox{ and } 2$ 

$$H = -t \sum_{\sigma} \left( c_{1,\sigma}^{\dagger} c_{2,\sigma} + c_{2,\sigma}^{\dagger} c_{1,\sigma} \right) + U \sum_{i=1}^{2} n_{i,\uparrow} n_{i,\downarrow}.$$

- This can be solved by exact diagonalization
- Generate all states of the Hilbert space with given electron numbers  $N_{\uparrow}$  and  $N_{\downarrow}$  on N lattice sites

$$n_{Basis} = \left(\begin{array}{c} N\\ N_{\uparrow} \end{array}\right) \cdot \left(\begin{array}{c} N\\ N_{\downarrow} \end{array}\right)$$

- Set up the Hamilton matrix in this basis and diagonalize it numerically
- Obtain physical observables from the solution

$$H = -t \sum_{\sigma} \left( c_{1,\sigma}^{\dagger} c_{2,\sigma} + c_{2,\sigma}^{\dagger} c_{1,\sigma} \right) + U \sum_{i=1}^{2} n_{i,\uparrow} n_{i,\downarrow}$$

- The dimer Hamiltonian is invariant under the exchange of the two sites  $1 \leftrightarrow 2$
- We can therefore classify states also by their parity  $P = \pm 1$  under this exchange
- We may also view the dimer as '2-site ring with periodic boundary conditions' and hopping integral  $\frac{t}{2}$



- Exchange of the sites is equaivalent to translation by one lattice site
- A Bloch state  $\psi_k$  with momentum k obeys  $T_1 \ \psi_k = e^{ik} \ \psi_k$

P=1 is equivalent to  $k=0,\,P=-1$  is equivalent to  $k=\pi$ 

- We start with the sector  $N_{\uparrow}=N_{\downarrow}=1$  'half filling' and nonmagnetic
- The normalized basis states with  $P = \pm 1$  are

$$\begin{aligned} |1_{\pm}\rangle &= \frac{1}{\sqrt{2}} \left( c_{1,\uparrow}^{\dagger} c_{2,\downarrow}^{\dagger} \pm c_{2,\uparrow}^{\dagger} c_{1,\downarrow}^{\dagger} \right) |0\rangle \\ |2_{\pm}\rangle &= \frac{1}{\sqrt{2}} \left( c_{1,\uparrow}^{\dagger} c_{1,\downarrow}^{\dagger} \pm c_{2,\uparrow}^{\dagger} c_{2,\downarrow}^{\dagger} \right) |0\rangle \end{aligned}$$

- $|1_+\rangle$  is spin singlet,  $|1_-\rangle$  is triplet (with  $S^z = 0$ ),  $|2_+\rangle$  and  $|2_-\rangle$  are singlets
- The action of the kinetic term is

$$\begin{split} H_t \left| 1_+ \right\rangle &= -t \sum_{\sigma} \left( c_{1,\sigma}^{\dagger} c_{2,\sigma} + c_{2,\sigma}^{\dagger} c_{1,\sigma} \right) \frac{1}{\sqrt{2}} \left( c_{1,\uparrow}^{\dagger} c_{2,\downarrow}^{\dagger} + c_{2,\uparrow}^{\dagger} c_{1,\downarrow}^{\dagger} \right) \left| 0 \right\rangle \\ &= \frac{-t}{\sqrt{2}} \left( \left( c_{2,\uparrow}^{\dagger} c_{2,\downarrow}^{\dagger} + c_{1,\uparrow}^{\dagger} c_{1,\downarrow}^{\dagger} \right) + \left( c_{1,\uparrow}^{\dagger} c_{1,\downarrow}^{\dagger} + c_{2,\uparrow}^{\dagger} c_{2,\downarrow}^{\dagger} \right) \right) \left| 0 \right\rangle \\ &= \frac{-2t}{\sqrt{2}} \left( c_{1,\uparrow}^{\dagger} c_{1,\downarrow}^{\dagger} + c_{2,\uparrow}^{\dagger} c_{2,\downarrow}^{\dagger} \right) = -2t \left| 2_+ \right\rangle \end{split}$$

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- The normalized basis states with  $P = \pm 1$  are

$$\begin{aligned} |1_{\pm}\rangle &= \frac{1}{\sqrt{2}} \left( c_{1,\uparrow}^{\dagger} c_{2,\downarrow}^{\dagger} \pm c_{2,\uparrow}^{\dagger} c_{1,\downarrow}^{\dagger} \right) |0\rangle \\ |2_{\pm}\rangle &= \frac{1}{\sqrt{2}} \left( c_{1,\uparrow}^{\dagger} c_{1,\downarrow}^{\dagger} \pm c_{2,\uparrow}^{\dagger} c_{2,\downarrow}^{\dagger} \right) |0\rangle \end{aligned}$$

•  $|1_+\rangle$  is spin singlet,  $|1_-\rangle$  is triplet (with  $S^z = 0$ ),  $|2_+\rangle$  and  $|2_-\rangle$  are singlets

= 0

• The action of the kinetic term is

$$\begin{split} H_t \left| 1_{-} \right\rangle &= -t \sum_{\sigma} \left( c_{1,\sigma}^{\dagger} c_{2,\sigma} + c_{2,\sigma}^{\dagger} c_{1,\sigma} \right) \frac{1}{\sqrt{2}} \left( c_{1,\uparrow}^{\dagger} c_{2,\downarrow}^{\dagger} - c_{2,\uparrow}^{\dagger} c_{1,\downarrow}^{\dagger} \right) \left| 0 \right\rangle \\ &= \frac{-t}{\sqrt{2}} \left( \left( c_{2,\uparrow}^{\dagger} c_{2,\downarrow}^{\dagger} + c_{1,\uparrow}^{\dagger} c_{1,\downarrow}^{\dagger} \right) - \left( c_{1,\uparrow}^{\dagger} c_{1,\downarrow}^{\dagger} + c_{2,\uparrow}^{\dagger} c_{2,\downarrow}^{\dagger} \right) \right) \left| 0 \right\rangle \end{split}$$

We had

$$H_t |1_+\rangle = -2t |2_+\rangle \implies \langle 2_+| H_t |1_+\rangle = -2t$$
$$H_t |1_-\rangle = 0 \implies \langle 2_-| H_t |1_-\rangle = 0$$

We recall

so that

$$|1_{\pm}\rangle = \frac{1}{\sqrt{2}} \left( c_{1,\uparrow}^{\dagger} c_{2,\downarrow}^{\dagger} \pm c_{2,\uparrow}^{\dagger} c_{1,\downarrow}^{\dagger} \right) |0\rangle \qquad \langle 1_{\pm} | H_U | 1_{\pm} \rangle = 0$$
  

$$|2_{\pm}\rangle = \frac{1}{\sqrt{2}} \left( c_{1,\uparrow}^{\dagger} c_{1,\downarrow}^{\dagger} \pm c_{2,\uparrow}^{\dagger} c_{2,\downarrow}^{\dagger} \right) |0\rangle \qquad \langle 2_{\pm} | H_U | 2_{\pm} \rangle = U$$

Writing  $|\psi_{\pm}\rangle = u|1_{\pm}\rangle + v|2_{\pm}\rangle$  the coefficients (u, v) are obtained from the eigenvalue problems

$$\begin{pmatrix} 0 & -2t \\ -2t & U \end{pmatrix} \begin{pmatrix} u_+ \\ v_+ \end{pmatrix} = E_+ \begin{pmatrix} u_+ \\ v_+ \end{pmatrix} \qquad \qquad \begin{pmatrix} 0 & 0 \\ 0 & U \end{pmatrix} \begin{pmatrix} u_- \\ v_- \end{pmatrix} = E_- \begin{pmatrix} u_- \\ v_- \end{pmatrix}$$

For negative parity the state with lower energy is  $|1_{-}\rangle$  with energy E = 0 - this  $|1_{-}\rangle$  is a triplet The other two members of the triplet are  $c_{1,\uparrow}^{\dagger}c_{2,\uparrow}^{\dagger} |0\rangle$  and  $c_{1,\downarrow}^{\dagger}c_{2,\downarrow}^{\dagger} |0\rangle$  - these are the only states in the sectors  $N_{e} = 2$ ,  $S_{z} = \pm 1$  and  $P = -1 \Rightarrow$  eigenstates by construction, energy E = 0

For positive parity the eigenvalue problem was

$$\begin{pmatrix} 0 & -2t \\ -2t & U \end{pmatrix} \begin{pmatrix} u_+ \\ v_+ \end{pmatrix} = E_+ \begin{pmatrix} u_+ \\ v_+ \end{pmatrix}$$

The lower state - which is a singlet - has energy

$$E_0 = \frac{U}{2} - \sqrt{\left(\frac{U}{2}\right)^2 + 4t^2} \xrightarrow{U/t \to \infty} \frac{U}{2} - \left(\frac{U}{2} + \frac{4t^2}{U}\right) = -\frac{4t^2}{U} = -J$$

The ground state is a singlet the first excited state a triplet with excitation energy  $J = \frac{4t^2}{U} \ll t$  (for  $U/t \gg 1$ )

To calculate the Green's function we need the eigenstates with 1 or 3 electrons,  $S_z = \sigma = \pm \frac{1}{2}$  and parity  $\pm 1$ (we recall: P = 1 means k = 0, P = -1 means  $k = \pi$ ):

$$\begin{aligned} |3_{\pm},\sigma\rangle &= \frac{1}{\sqrt{2}} \left( c_{1,\sigma}^{\dagger} \pm c_{2,\sigma}^{\dagger} \right) |0\rangle, \\ |4_{\pm},\sigma\rangle &= \frac{1}{\sqrt{2}} \left( c_{1,\sigma}^{\dagger} c_{2,\uparrow}^{\dagger} c_{2,\downarrow}^{\dagger} \pm c_{2,\sigma}^{\dagger} c_{1,\uparrow}^{\dagger} c_{1,\downarrow}^{\dagger} \right) |0\rangle. \end{aligned}$$

• These states are the only ones in their respective  $(N_e, S_z, P)$  sector  $\Rightarrow$  eigenstates by construction

• Their energies are (with 
$$\epsilon_k = -t \cos(k)$$
)

$$H |3_{\pm}, \sigma\rangle = \mp t |3_{\pm}, \sigma\rangle = \epsilon_k |3_{\pm}, \sigma\rangle$$
$$H |4_{\pm}, \sigma\rangle = (U \pm t) |4_{\pm}, \sigma\rangle = (U - \epsilon_k) |4_{\pm}, \sigma\rangle$$

We thus know all eigenstates  $|j\rangle$  with  $N_e = 0, 1, 2, 3, 4$  as well as their energies  $E_j$ We can now evaluate the Green's function using the Lehmann representation  $(k = 0, \pi)$ :

$$G(k,\omega) = \frac{1}{Z} \sum_{i,j} \frac{e^{-\beta(E_i - \mu N_i)} + e^{-\beta(E_j - \mu N_j)}}{\omega + \mu - (E_j - E_i)} |\langle i| \ c_k |j\rangle|^2$$

with

$$c_{k,\sigma} = \frac{1}{\sqrt{2}} \left( c_{1,\sigma} \pm c_{2,\sigma} \right)$$

From the Green's function we can then obtain the self-energy  $\Sigma(k,\omega)$  from the Dyson equation

$$(\omega + \mu - \epsilon_k - \Sigma(k, \omega)) G(k, \omega) = 1.$$

For simplicity we consider the limit of low temperature and assume that  $\mu$  is chosen such that the thermal occupation factor  $e^{-\beta(E_j-\mu N_j)}/Z$  is 1 for the ground state with 2 electrons and 0 otherwise (this can in fact be achieved by choosing  $\mu = \frac{U}{2}$  and  $T \ll J$ )

In this limit we can actually give analytical expressions for G and  $\Sigma$ 

$$G(k,\omega) = \frac{\frac{1}{2} - \frac{\epsilon_k}{W}}{\omega + \mu - (E_0 - \epsilon_k)} + \frac{\frac{1}{2} + \frac{\epsilon_k}{W}}{\omega + \mu - (U - \epsilon_k - E_0)}$$

$$E_0 = \frac{U}{2} - W$$

$$W = \sqrt{\left(\frac{U}{2}\right)^2 + 4t^2}$$

$$\Sigma(k,\omega) = \frac{U}{2} + \frac{\left(\frac{U}{2}\right)^2}{\omega + \mu + 3\epsilon_k - \frac{U}{2}} = V_{HF} + \sum_{i=1}^{1} \frac{\sigma_i}{\omega - \zeta_i}$$

In this limit we can actually give analytical expressions for G and  $\Sigma$ 

$$\begin{split} G(k,\omega) &= \frac{\frac{1}{2} - \frac{\epsilon_k}{W}}{\omega + \mu - (E_0 - \epsilon_k)} + \frac{\frac{1}{2} + \frac{\epsilon_k}{W}}{\omega + \mu - (U - \epsilon_k - E_0)} \stackrel{U/t \to \infty}{\longrightarrow} \frac{\frac{1}{2} - \frac{2\epsilon_k}{U}}{\omega + \frac{U}{2} + \epsilon_k} + \frac{\frac{1}{2} + \frac{2\epsilon_k}{U}}{\omega - \frac{U}{2} + \epsilon_k} \\ E_0 &= \frac{U}{2} - W \stackrel{U/t \to \infty}{\longrightarrow} -\frac{4t^2}{U} \\ W &= \sqrt{\left(\frac{U}{2}\right)^2 + 4t^2} \stackrel{U/t \to \infty}{\longrightarrow} \frac{U}{2} + \frac{4t^2}{U} \\ \Sigma(k,\omega) &= \frac{U}{2} + \frac{\left(\frac{U}{2}\right)^2}{\omega + \mu + 3\epsilon_k - \frac{U}{2}} \stackrel{U/t \to \infty}{\longrightarrow} \frac{U}{2} + \frac{\left(\frac{U}{2}\right)^2}{\omega + 3\epsilon_k} \end{split}$$

Dimer spectrum compared to spectra of half-filled 16- and 18-site clusters (U/t = 10, Dots:  $-\epsilon_k$ )



$$\Sigma(\omega) = \frac{\sigma}{\omega - \zeta}$$

The equation for poles of the Green's function (=energies of electron states) reads:  $\omega - \epsilon_{\mathbf{k}} = \Sigma(\omega)$ 



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$$\omega_1 - \omega_2 = \sqrt{(\epsilon_k - \zeta)^2 + 4\sigma} \approx \sqrt{4\sigma} \Rightarrow \sigma \approx \frac{U^2}{2}$$

Dimer spectrum compared to spectra of 16- and 18-site clusters (U/t = 10)





## Summary, Hubbard Dimer

- At or close to half-filling: antiferromagnetic spin correlations, electrons on neighboring sites prefer to couple their spins to a singlet, or be antiparallel
- Spin excitations with new low energy scale  $J = \frac{4t^2}{U} \ll t$
- Photoemission/inverse photoemission spectrum shows Hubbard gap of order U
- This is 'pushed open' by a single pole of the self-energy with residuum  $\propto U^2$
- 'Gap-opening pole' has substantial dispersion  $\mathbf{k}$ -dependent self-energy
- Conjecture: residuum of 'gap-opening pole' would be natural order parameter for paramagnetic MIT:



### The Hubbard-I approximation

- We consider the Hubbard model at half-filling,  $N_e = N$ , and the nonmagnetic case  $N_{\uparrow} = N_{\downarrow} = N/2$
- We set t = 0, U finite
- The GS has one electron/site and is highly degenerate

$$n_{deg} = \left(\begin{array}{c} N\\ N/2 \end{array}\right)$$

- We ignore this degeneracy and assume that there is a single ground state  $|\Psi_0
  angle$
- $|\Psi_0
  angle$  may be thought of as a superposition of all the degenerate states with one electron per site
- Our main assumption is that  $|\Psi_0
  angle$  is 'disordered'
- Next we assume that a finite  $t \ll U$  is switched on
- This will result in charge fluctuations

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 $H = \sum_{i,j} \sum_{\sigma} \frac{t_{i,j}}{2} \left( d_{i,\sigma}^{\dagger} h_{j,-\sigma}^{\dagger} + H.c. \right) + \sum_{i,j} \sum_{\sigma} \frac{t_{i,j}}{2} \left( d_{i,\sigma}^{\dagger} d_{j,\sigma} - h_{i,-\sigma}^{\dagger} h_{j,-\sigma} \right) + U \sum_{i,\sigma} d_{i,\sigma}^{\dagger} d_{i,\sigma}$ 

Fourier transformation gives

$$H = \sum_{\mathbf{k},\sigma} \left( \left( \frac{\epsilon_{\mathbf{k}}}{2} + U \right) d_{\mathbf{k},\sigma}^{\dagger} d_{\mathbf{k},\sigma} - \frac{\epsilon_{\mathbf{k}}}{2} h_{\mathbf{k},\sigma}^{\dagger} h_{\mathbf{k},\sigma} \right) + \sum_{\mathbf{k},\sigma} \frac{\epsilon_{\mathbf{k}}}{2} \left( d_{\mathbf{k},\sigma}^{\dagger} h_{-\mathbf{k},-\sigma}^{\dagger} + H.c. \right)$$

This is a quadratic form which can be solved by a unitary transformation

$$\gamma_{-,\mathbf{k},\sigma} = u_{\mathbf{k}} d_{\mathbf{k},\sigma} + v_{\mathbf{k}} h^{\dagger}_{-\mathbf{k},-\sigma}$$
  

$$\gamma_{+,\mathbf{k},\sigma} = -v_{\mathbf{k}} d_{\mathbf{k},\sigma} + u_{\mathbf{k}} h^{\dagger}_{-\mathbf{k},-\sigma}$$
(1)

Demanding...

$$[H, \gamma^{\dagger}_{\alpha, \mathbf{k}, \sigma}] = E_{\mathbf{k}} \gamma^{\dagger}_{\alpha, \mathbf{k}, \sigma}$$

... leads to the eigenvalue problem

$$\begin{pmatrix} \frac{\epsilon_{\mathbf{k}}}{2} & , & \frac{\epsilon_{\mathbf{k}}}{2} \\ \frac{\epsilon_{\mathbf{k}}}{2} & , & \frac{\epsilon_{\mathbf{k}}}{2} + U \end{pmatrix} \begin{pmatrix} u_{\mathbf{k}} \\ v_{\mathbf{k}} \end{pmatrix} = E_{\mathbf{k}} \begin{pmatrix} u_{\mathbf{k}} \\ v_{\mathbf{k}} \end{pmatrix}$$

This is readily solved to give the energies of the two Hubbard bands

$$E_{\mathbf{k},\pm} = \frac{1}{2} \left( \epsilon_{\mathbf{k}} + U \pm \sqrt{\epsilon_{\mathbf{k}}^2 + U^2} \right) \stackrel{U/t \to \infty}{\longrightarrow} \begin{cases} \frac{\epsilon_{\mathbf{k}}}{2} + U \\ \frac{\epsilon_{\mathbf{k}}}{2} \end{cases}$$

Example: U/t = 10

Particle-hole-symmetry :  $\mu = U/2 = 5$ 

Comparison with Hartree-approximation:

$$E_{\mathbf{k}} = \frac{U}{2} + \epsilon_{\mathbf{k}}$$



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 $H = \sum_{i,j} \sum_{\sigma} \frac{t_{i,j}}{2} \left( d_{i,\sigma}^{\dagger} h_{j,-\sigma}^{\dagger} + H.c. \right) + \sum_{i,j} \sum_{\sigma} \frac{t_{i,j}}{2} \left( d_{i,\sigma}^{\dagger} d_{j,\sigma} - h_{i,-\sigma}^{\dagger} h_{j,-\sigma} \right) + U \sum_{i,\sigma} d_{i,\sigma}^{\dagger} d_{i,\sigma}$ 

We split the electron annihilation operator into the part which reduces the number of double occupancies by one and the part which leaves the number of double occupancies constant

 $\hat{d}_{i,\uparrow}$  and  $\hat{c}_{i,\uparrow}$  are called Hubbard operators



Accordingly these operators obey

$$[\hat{d}_{i,\sigma}, H_U] = U \ \hat{d}_{i,\sigma} \qquad [\hat{c}_{i,\sigma}, H_U] = 0$$

The time ordered Green's functions for these operators is (with  $\alpha, \beta \in {\hat{c}, \hat{d}}$ )

$$G_{\alpha,\beta}({\bf k},t) \;=\; -i \langle \; T \; \alpha_{{\bf k},\sigma}(t) \; \beta_{{\bf k},\sigma}^{\dagger} \; \rangle$$

These obey the equations of motion

$$i\partial_t G_{\alpha,\beta}(\vec{k},t) = \delta(t) \langle \{\beta^{\dagger}_{\mathbf{k},\sigma}, \alpha_{\mathbf{k},\sigma}\} \rangle - i \langle T [\alpha_{\mathbf{k},\sigma}, H](t) \beta^{\dagger}_{\mathbf{k},\sigma} \rangle.$$

Consider the hopping term between the sites i and j:  $T_{i,j} = t_{i,j} \sum_{\sigma} \left( c_{i,\sigma}^{\dagger} c_{j,\sigma} + c_{j,\sigma}^{\dagger} c_{i,\uparrow} \right)$  with

$$[c_{i,\sigma}, T_{i,j}] = t_{i,j} c_{j,\sigma} \qquad [c_{i,\sigma}^{\dagger}, T_{i,j}] = -t_{i,j} c_{j,\sigma}^{\dagger}$$

Then (remember:  $\hat{c}_{i,\uparrow} = c_{i,\uparrow} (1 - n_{i,\downarrow}) = c_{i,\uparrow} c_{i,\downarrow} c_{i,\downarrow}^{\dagger}$ )

$$\begin{split} \left[ \hat{c}_{i,\uparrow}, T_{i,j} \right] &= \left[ c_{i,\uparrow} \ c_{i,\downarrow} \ c_{i,\downarrow}^{\dagger} \ , \ T_{i,j} \right] \\ &= c_{i,\uparrow} \ c_{i,\downarrow} \ \left[ c_{i,\downarrow}^{\dagger}, T_{i,j} \right] + c_{i,\uparrow} \ \left[ c_{i,\downarrow}, T_{i,j} \right] \ c_{i,\downarrow}^{\dagger} + \left[ c_{i,\uparrow}, T_{i,j} \right] \ c_{i,\downarrow} \ c_{i,\downarrow}^{\dagger} \\ &= t_{i,j} (-c_{i,\uparrow} \ c_{i,\downarrow} \ c_{j,\downarrow}^{\dagger} + c_{i,\uparrow} \ c_{j,\downarrow} \ c_{i,\downarrow}^{\dagger} + c_{j,\uparrow} \ c_{i,\downarrow} \ c_{i,\downarrow}^{\dagger} ) \\ &= t_{i,j} (-c_{i,\uparrow} \ c_{i,\downarrow} \ c_{j,\downarrow}^{\dagger} + c_{i,\uparrow}^{\dagger} \ c_{j,\downarrow} + c_{j,\uparrow} \ (1 - n_{i,\downarrow}) ) ) \\ &= t_{i,j} (-c_{i,\uparrow} \ c_{i,\downarrow} \ c_{j,\downarrow}^{\dagger} + S_i^{-} \ c_{j,\downarrow} + c_{j,\uparrow} \ (1 - (\frac{n_i}{2} - S_i^z)) ) ) \\ &= t_{i,j} (-c_{i,\uparrow} \ c_{i,\downarrow} \ c_{j,\downarrow}^{\dagger} + (S_i^{-} \ c_{j,\downarrow} + S_i^z \ c_{j,\uparrow} ) + c_{j,\uparrow} \ (1 - (\frac{n_i}{2}) - (\frac{n_i}{2} - \frac{\langle n_i \rangle}{2} ) ) \end{split}$$

Collecting terms and writing  $\langle n_i \rangle = n_e$  we find

$$\begin{bmatrix} \hat{c}_{i,\uparrow}, H_t \end{bmatrix} = \sum_j t_{ij} \left[ (1 - \frac{n_e}{2}) c_{j,\uparrow} + (c_{j,\uparrow} S_i^z + c_{j,\downarrow} S_i^-) - \frac{1}{2} c_{j,\uparrow} (n_i - n_e) + c_{j,\downarrow}^{\dagger} c_{i,\downarrow} c_{i,\downarrow} c_{i,\uparrow} \right]$$

$$\begin{bmatrix} \hat{d}_{i,\uparrow}, H_t \end{bmatrix} = \sum_j t_{ij} \left[ \frac{n_e}{2} c_{j,\uparrow} - (c_{j,\uparrow} S_i^z + c_{j,\downarrow} S_i^-) + \frac{1}{2} c_{j,\uparrow} (n_i - n_e) - c_{j,\downarrow}^{\dagger} c_{i,\downarrow} c_{i,\downarrow} c_{i,\uparrow} \right]$$

The various terms describe

Coherent propagation from  $i \rightarrow j$  with reduced hopping element

Hopping  $i \rightarrow j$  while leaving a spin excitation at i

Hopping  $i \rightarrow j$  while leaving a density excitation at i

Hopping  $i \rightarrow j$  while leaving a pair excitation at i (important only for U < 0)

The Hubbard-I approximation corresponds to a rather crude truncation:

$$[\hat{c}_{i,\uparrow}, H_t] = \sum_j t_{ij} (1 - \frac{n_e}{2}) c_{j,\uparrow} = (1 - \frac{n_e}{2}) \sum_j t_{ij} (\hat{c}_{j,\uparrow} + \hat{d}_{j,\uparrow})$$
$$[\hat{d}_{i,\uparrow}, H_t] = \sum_j t_{ij} \frac{n_e}{2} c_{j,\uparrow} = \frac{n_e}{2} \sum_j t_{ij} (\hat{c}_{j,\uparrow} + \hat{d}_{j,\uparrow})$$

Spatial Fourier transformation and adding the commutator with  $H_U$  gives

$$\begin{bmatrix} \hat{c}_{\mathbf{k},\uparrow}, H \end{bmatrix} = (1 - \frac{n_e}{2}) \epsilon_{\mathbf{k}} \left( \hat{c}_{\mathbf{k},\uparrow} + \hat{d}_{\mathbf{k},\uparrow} \right)$$
$$\begin{bmatrix} \hat{d}_{\mathbf{k},\uparrow}, H \end{bmatrix} = \frac{n_e}{2} \epsilon_{\mathbf{k}} \left( \hat{c}_{\mathbf{k},\uparrow} + \hat{d}_{\mathbf{k},\uparrow} \right) + U \hat{d}_{\mathbf{k},\uparrow}$$

The anticommutators are (remember:  $\hat{c}^{\dagger}_{i,\sigma} = c^{\dagger}_{i,\sigma} \; (1 - n_{i-\sigma})$ )

$$\{ \hat{c}_{i,\sigma}^{\dagger}, \hat{c}_{i,\sigma} \} = \{ c_{i,\sigma}^{\dagger}, c_{i,\sigma} \} (1 - n_{i-\sigma})^2 = 1 - n_{i-\sigma}$$
$$\{ \hat{d}_{i,\sigma}^{\dagger}, \hat{d}_{i,\sigma} \} = n_{i-\sigma}$$

Now we have every ingredient to set up the equations of motion

$$i\partial_t G_{\alpha,\beta}(\vec{k},t) = \delta(t) \langle \{\beta_{\mathbf{k},\sigma}^{\dagger}, \alpha_{\mathbf{k},\sigma}\} \rangle - i \langle T[\alpha_{\mathbf{k},\sigma}, H](t) \beta_{\mathbf{k},\sigma}^{\dagger} \rangle.$$

For example  $\alpha = \hat{d}$ ,  $\beta = \hat{d}$ :

$$i\partial_t \ G_{\hat{d},\hat{d}}(\vec{k},t) \ = \ \delta(t) \ \langle n_{-\sigma} \rangle + \frac{n_e}{2} \ \epsilon_{\mathbf{k}} \left( \ G_{\hat{c},\hat{d}}(\vec{k},t) + \ G_{\hat{d},\hat{d}}(\vec{k},t) \right) + \frac{U}{U} \ G_{\hat{d},\hat{d}}(\vec{k},t)$$
After Fourier transformation with respect to time  $(i\partial_t \to \omega)$  we obtain the system of equations

$$\begin{pmatrix} \omega - (1 - \frac{n_e}{2}) \epsilon_{\mathbf{k}} , -(1 - \frac{n_e}{2}) \epsilon_{\mathbf{k}} \\ -\frac{n_e}{2} \epsilon_{\mathbf{k}} , \omega - \frac{n_e}{2} \epsilon_{\mathbf{k}} - U \end{pmatrix} \begin{pmatrix} G_{\hat{c},\hat{c}} & G_{\hat{c},\hat{d}} \\ G_{\hat{d},\hat{c}} & G_{\hat{d},\hat{d}} \end{pmatrix} = \begin{pmatrix} 1 - \frac{n_e}{2} , 0 \\ 0 , \frac{n_e}{2} \end{pmatrix}$$

Now we can use ....

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix}^{-1} = \frac{1}{ad - bc} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix}$$

... to solve for the  $2 \times 2$  matrix  $\mathbf{G}(\mathbf{k}, \omega)$ 

Since  $c_{{\bf k},\sigma}=\hat{c}_{{\bf k},\sigma}+\hat{d}_{{\bf k},\sigma}$  the electron Green's function

$$G(\mathbf{k},t) = -i\langle Tc_{\mathbf{k},\sigma}(t) c^{\dagger}_{\mathbf{k},\sigma} \rangle,$$

can be obtained as  $G = G_{\hat{c},\hat{c}} + G_{\hat{c},\hat{d}} + G_{\hat{d},\hat{c}} + G_{\hat{d},\hat{d}}$ 

After some algebra this can be brought to the familiar-looking form...

$$G(\mathbf{k},\omega) = \frac{1}{\omega - \epsilon_{\mathbf{k}} - \Sigma(\omega)}$$

...where the k-independent self-energy  $\Sigma(\omega)$  is given by

$$\Sigma(\omega) = \frac{n_e}{2} U + \frac{n_e}{2} \left(1 - \frac{n_e}{2}\right) \frac{U^2}{\omega - \left(1 - \frac{n_e}{2}\right) U}$$
$$= V_{HF} + \frac{\sigma}{\omega - \zeta}$$

 $\Rightarrow$  Sum of Hartree-Fock potential and a single term with a pole - as established by Luttinger

First check: Comparison to exact spectra for the dimer

Simply use 'dimer dispersion'  $\epsilon_k = -t \cos(k)$  and the Hubbard-I self-energy for  $n_e = 1$  in the Dyson equation

A(k,ω) .....  $A(k,\omega)$  $\Sigma(k,\omega)$  $\Sigma(k,\omega)$ k=π Intensity [arb. u.] Intensity [arb. u.] k=π k=0 k=0 -10 -5 5 -10 -5 5 10 0 10 0 (w–U/2)/t ω/t

Exact

Hubbard-I





Note the transfer of spectral weight upon decreasing electron density

(Experimental data on La<sub>2-x</sub>Sr<sub>x</sub>CuO<sub>4</sub> by C.T. Chen *et al.*, Phys. Rev. Lett. 66, 104 (1991))

For small doping the Fermi surface is a small pocket around  $(\pi, \pi)$  - the Fermi surface volume depends on electron density in a strange nonlinear way - this is a well-known deficiency of the Hubbard-I approximation



Comparison to  $A(\mathbf{k}, \omega)$  obtained by QMC on an  $8 \times 8$  cluster, U/t = 8,  $n_e = 1$ C. Gröber *et al*, PRB **62**, 4336 (2000).



QMC at  $k_BT = t$  - Fermi surface volume



Rough estimate for fractional Fermi surface volume

$$V_{Fermi} = \frac{1}{64} \sum_{\mathbf{k}} n_{\mathbf{k}},$$



## Summary: the Hubbard-I approximation

- Basic physical idea: consider half-filled state as 'vacuum'
  - interpret charge fluctuations as hole-like and double occupany-like 'particles'
- The particles have energies 0 and  $U \Rightarrow$  two Hubbard-bands
- Self-energy has a single dispersionless 'gap opening peak' with residuum  $\propto U^2$  (*cave* exact diagonalization!)
- At half-filling ( $n_e = 1$ ): lower Hubbard band is filled completely
- Less than half-filling: lower Hubbard band is 'hole doped'
- Fermi surface is a small hole pocket at the maximum of the lower Hubbard band (usually  $(\pi,\pi)$ )
- Hole-pocket volume  $\rightarrow 0$  as  $n_e \rightarrow 1$  MIT by vanishing carrier density
- Strange nonlinear dependence of Fermi surface volume on electron density
- Comparison with QMC: soso....

### The Gutzwiller wave function

Basic idea: With increasing U/t the probability to find doubly occupied sites will decrease This may be described by the following variational wave function

$$|\Phi_G\rangle = \prod_i (1 - \lambda n_{i,\uparrow} n_{i,\downarrow}) |FS\rangle$$

- $|FS\rangle$  is the free electron ground state i.e. the Fermi sea
- $\lambda$  is a variational parameter to be determined from  $\langle \Phi_G | H | \Phi_G \rangle / \langle \Phi_G | \Phi_G \rangle \rightarrow min$

The operator  $1-\lambda \; n_{\uparrow}n_{\downarrow}$  acts like this

$(1-\lambda \; n_{\uparrow}n_{\downarrow})$	$ 0\rangle$	=	$ 0\rangle$
$(1 - \lambda \; n_{\uparrow} n_{\downarrow})$	$ \uparrow\rangle$	=	$ \uparrow\rangle$
$(1 - \lambda \; n_{\uparrow} n_{\downarrow})$	$ \downarrow\rangle$	=	$ \downarrow angle$
$(1 - \lambda \ n_{\uparrow} n_{\downarrow})$	$ \uparrow\downarrow angle$	=	$(1-\lambda) \uparrow\downarrow\rangle$

A state with  $N_d$  double occupancies gets a factor of  $(1-\lambda)^{N_d} \ll 1$ 

Rewriting the Fermi sea  $|FS\rangle$ 

We use (spin index suppressed!)

$$c_{\mathbf{k}}^{\dagger} = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} e^{i\mathbf{k}\cdot\mathbf{R}_{j}} c_{j}^{\dagger}$$

Then

$$\prod_{j=1}^{M} c_{\mathbf{k}_{j}}^{\dagger} |0\rangle = \frac{1}{\sqrt{N}^{M}} \sum_{i_{1}, i_{2}, i_{3}, \dots i_{M}} exp\left(i \sum_{j=1}^{M} \mathbf{k}_{j} \cdot \mathbf{R}_{i_{j}}\right) c_{i_{1}}^{\dagger} c_{i_{2}}^{\dagger} \dots c_{i_{M}}^{\dagger} |0\rangle$$

## Here we sum over all M-tuples of site indices

We may as well sum over all ordered M-tuples and then sum over all permutations of M indizes

$$\prod_{j=1}^{M} c_{\mathbf{k}_{j}}^{\dagger} |0\rangle = \frac{1}{\sqrt{N}^{M}} \sum_{i_{1}>i_{2}>i_{3}\cdots>i_{M}} \sum_{\sigma} exp\left(i\sum_{j=1}^{M} \mathbf{k}_{j} \cdot \mathbf{R}_{i_{\sigma(j)}}\right) c_{i_{\sigma(1)}}^{\dagger} c_{i_{\sigma(2)}}^{\dagger} \dots c_{i_{\sigma(M)}}^{\dagger} |0\rangle$$

We had

$$\prod_{j=1}^{M} c_{\mathbf{k}_{j}}^{\dagger} |0\rangle = \frac{1}{\sqrt{N}^{M}} \sum_{i_{1}>i_{2}>i_{3}\cdots>i_{M}} \sum_{\sigma} exp\left(i\sum_{j=1}^{M} \mathbf{k}_{j} \cdot \mathbf{R}_{i_{\sigma(j)}}\right) c_{i_{\sigma(1)}}^{\dagger} c_{i_{\sigma(2)}}^{\dagger} \dots c_{i_{\sigma(M)}}^{\dagger} |0\rangle$$

The product of creation operators can be brought back to the original ordered sequence

$$c_{i_{\sigma(1)}}^{\dagger}c_{i_{\sigma(2)}}^{\dagger}\dots c_{i_{\sigma(M)}}^{\dagger}|0\rangle = (-1)^{\sigma'}c_{i_1}^{\dagger}c_{i_2}^{\dagger}\dots c_{i_M}^{\dagger}|0\rangle$$

Since obviously  $\sigma'=\sigma^{-1}$  we have  $(-1)^{\sigma'}=(-1)^{\sigma}$  we finally have

$$\begin{split} \prod_{j=1}^{M} c_{\mathbf{k}_{j}}^{\dagger} \left| 0 \right\rangle &= \frac{1}{\sqrt{N}^{M}} \sum_{i_{1} > i_{2} > i_{3} \cdots > i_{M}} \sum_{\sigma} (-1)^{\sigma} exp\left( i \sum_{j=1}^{M} \mathbf{k}_{j} \cdot \mathbf{R}_{i_{\sigma}(j)} \right) c_{i_{1}}^{\dagger} c_{i_{2}}^{\dagger} c_{i_{M}}^{\dagger} \left| 0 \right\rangle \\ &= \frac{1}{\sqrt{N}^{M}} \sum_{i_{1} > i_{2} > i_{3} \cdots > i_{M}} D(\mathbf{k}_{1}, \mathbf{k}_{2}, \dots, \mathbf{k}_{M} | i_{1}, i_{2}, \dots, i_{M}) \quad c_{i_{1}}^{\dagger} c_{i_{2}}^{\dagger} c_{i_{M}}^{\dagger} \left| 0 \right\rangle \end{split}$$

Assuming this procedure carried out for both spin directions, the Fermi sea  $|FS\rangle$  therefore may be thought of as the superposition of all real space configurations

$$D(\mathbf{k}_1,\ldots,\mathbf{k}_{N_{\uparrow}}|i_1,\ldots,i_{N_{\uparrow}}) \ D(\mathbf{k}'_1,\ldots,\mathbf{k}'_{N_{\downarrow}}|j_1,\ldots,j_{N_{\downarrow}}) \ c^{\dagger}_{i_1,\uparrow}\ldots c^{\dagger}_{i_{N_{\uparrow}},\uparrow} \ c^{\dagger}_{j_1,\downarrow}\ldots c^{\dagger}_{j_{N_{\downarrow}},\downarrow} \ |0\rangle$$

In the Gutzwiller wave function each of these configurations gets an additional factor of  $(1 - \lambda)^{N_d} < 1$  where  $N_d$  is the number of sites belonging to  $\{i_1, \ldots i_{N_{\uparrow}}\} \cap \{j_1, \ldots j_{N_{\downarrow}}\}$ 

Why do we insist on ordered M-tuples  $(i_1, \ldots i_{N_{\uparrow}})$  and  $(j_1, \ldots j_{N_{\downarrow}})$ ?

Because then each real-space configuration of electrons is included only once and all real space configurations are mutually orthogonal

The Gutzwiller wave function can be decomposed into components with fixed number of double occupancies

$$|\Phi_G\rangle = \sum_{N_d} |\Phi(N_d)\rangle$$

$$|\Phi(0)\rangle = a \begin{vmatrix} \phi & \phi \\ \phi & \phi \\ \phi & \phi \end{vmatrix} + b \begin{vmatrix} \phi & \phi \\ \phi & \phi \\ \phi & \phi \end{vmatrix} + c \begin{vmatrix} \phi & \phi \\ \phi & \phi \\ \phi & \phi \end{vmatrix} + \dots$$

$$|\Phi(1)\rangle = d \begin{vmatrix} \phi & \phi \\ \phi & \circ \end{vmatrix} + e \begin{vmatrix} \phi & \phi \\ \circ & \phi \end{vmatrix} + f \begin{vmatrix} \circ & \phi \\ \phi & \phi \end{vmatrix} + \dots$$

$$|\Phi(2)\rangle = g \left[ \begin{array}{c} \downarrow \downarrow \\ \downarrow \downarrow \\ \circ \\ \circ \\ \end{array} \right] + k \left[ \begin{array}{c} \circ \\ \downarrow \downarrow \\ \circ \\ \circ \\ \downarrow \downarrow \\ \end{array} \right] + h \left[ \begin{array}{c} \downarrow \downarrow \\ \circ \\ \circ \\ \downarrow \downarrow \\ \end{array} \right] + \dots$$

The Gutzwiller wave function can be decomposed into components with fixed number of double occupancies

$$|\Phi_G\rangle = \sum_{N_d} |\Phi(N_d)\rangle$$

Since the overlap of any two states with different  $N_d$  is zero we have

$$\langle \Phi_G | \Phi_G \rangle = \sum_{N_d} \langle \Phi(N_d) | \Phi(N_d) \rangle = \sum_{N_d} W(N_d)$$

Question: Which  $N_d$  has the largest weight  $W(N_d)$  in this sum?

 $W(N_d)$  obviously is the probability distribution for the number of double occupancies in the Gutzwiller wave function

Therefore the question may also be stated as: Which number of double occupancies is the most probable one?

Remember:  $|\Phi(N_d)\rangle$  is the sum over all ordered  $N_{\uparrow}$ -tuples  $i_1, i_2, \dots i_{N_{\uparrow}}$  and  $N_{\downarrow}$ -tuples  $j_1, j_2, \dots j_{N_{\downarrow}}$  of

$$D(\mathbf{k}_1,\ldots,\mathbf{k}_{N_{\uparrow}}|i_1,\ldots,i_{N_{\uparrow}}) \ D(\mathbf{k}'_1,\ldots,\mathbf{k}'_{N_{\downarrow}}|j_1,\ldots,j_{N_{\downarrow}}) \ c^{\dagger}_{i_1,\uparrow}\ldots c^{\dagger}_{i_{N_{\uparrow}},\uparrow} \ c^{\dagger}_{j_1,\downarrow}\ldots c^{\dagger}_{j_{N_{\downarrow}},\downarrow} \ |0\rangle$$

such that  $\{i_1, \ldots i_{N_{\uparrow}}\} \cap \{j_1, \ldots j_{N_{\downarrow}}\}$  comprises  $N_d$  sites - additional prefactor:  $(1 - \lambda)^{N_d} \frac{1}{\sqrt{N^{N_{\uparrow}+N_{\downarrow}}}}$ Since any two configurations are orthogonal we only need  $D^*(\mathbf{k_j}|i_j) D(\mathbf{k_j}|i_j)$ 

$$D(\mathbf{k}_{1}, \mathbf{k}_{2}, \dots, \mathbf{k}_{M} | i_{1}, i_{2}, \dots, i_{M}) = \sum_{\sigma} (-1)^{\sigma} exp\left(i \sum_{j=1}^{M} \mathbf{k}_{j} \cdot \mathbf{R}_{i_{\sigma(j)}}\right)$$
$$D^{*}(\mathbf{k}_{j} | i_{j}) D(\mathbf{k}_{j} | i_{j}) = \sum_{\sigma, \sigma'} (-1)^{\sigma} (-1)^{\sigma'} exp\left(i \sum_{j=1}^{M} \mathbf{k}_{j} \cdot (\mathbf{R}_{i_{\sigma(j)}} - \mathbf{R}_{i_{\sigma'(j)}})\right)$$
$$= \sum_{\sigma} 1 + \sum_{\sigma \neq \sigma'} (-1)^{\sigma} (-1)^{\sigma'} exp\left(i \sum_{j=1}^{M} \mathbf{k}_{j} \cdot (\mathbf{R}_{i_{\sigma(j)}} - \mathbf{R}_{i_{\sigma'(j)}})\right)$$
$$= M!$$

# We want to calculate $\langle \Phi(N_d) | \Phi(N_d) \rangle$

Remember:  $|\Phi(N_d)\rangle$  is the sum over all ordered  $N_{\uparrow}$ -tuples  $i_1, i_2, \ldots i_{N_{\uparrow}}$  and  $N_{\downarrow}$ -tuples  $j_1, j_2, \ldots j_{N_{\downarrow}}$  of

$$D(\mathbf{k}_1,\ldots,\mathbf{k}_{N_{\uparrow}}|i_1,\ldots,i_{N_{\uparrow}}) D(\mathbf{k}'_1,\ldots,\mathbf{k}'_{N_{\downarrow}}|j_1,\ldots,j_{N_{\downarrow}}) c^{\dagger}_{i_1,\uparrow}\ldots c^{\dagger}_{i_{N_{\uparrow}},\uparrow} c^{\dagger}_{j_1,\downarrow}\ldots c^{\dagger}_{j_{N_{\downarrow}},\downarrow} |0\rangle$$

such that  $\{i_1, \ldots i_{N_{\uparrow}}\} \cap \{j_1, \ldots j_{N_{\downarrow}}\}$  comprises  $N_d$  sites - additional prefactor:  $(1 - \lambda)^{N_d} \frac{1}{\sqrt{N^{N_{\uparrow}+N_{\downarrow}}}}$ We have just seen that

$$D^*(\mathbf{k_j}|i_j) D(\mathbf{k_j}|i_j) = M!$$

The total weight of all states with  $N_d$  double occupancies therefore is the norm of each state times the number of states

$$W(N_d) = \langle \Phi(N_d) | \Phi(N_d) \rangle = \frac{N_{\uparrow}! N_{\downarrow}!}{N^{N_{\uparrow}+N_{\downarrow}}} (1-\lambda)^{2N_d} C(N_{\uparrow}, N_{\downarrow}, N_d)$$

 $C(N_{\uparrow}, N_{\downarrow}, N_{d})$ : number of ways in which  $N_{\uparrow}$   $\uparrow$ -electrons and  $N_{\downarrow} \downarrow$ -electrons can be distributed over the N lattice sites such as to generate  $N_{d}$  double occupancies

We seek:  $C(N_{\uparrow}, N_{\downarrow}, N_d)$ : the number of ways in which  $N_{\uparrow}$   $\uparrow$ -electrons and  $N_{\downarrow} \downarrow$ -electrons can be distributed over the N lattice sites such as to generate  $N_d$  double occupancies

All in all we have N sites - these N sites have to be divided into

- $N_d$  sites with double occupancy
- $N_{\uparrow} N_d$  sites with  $\uparrow$ -electron only
- $N_{\downarrow} N_d$  sites with  $\downarrow$ -electron only

•  $N - N_d - (N_{\uparrow} - N_d) - (N_{\downarrow} - N_d) = N - N_{\uparrow} - N_{\downarrow} + N_d$  empty sites

The answer then is the multinomial coefficient

$$C(N_{\uparrow}, N_{\downarrow}, N_d) = \frac{N!}{N_d! (N_{\uparrow} - N_d)! (N_{\downarrow} - N_d)! (N - N_{\uparrow} - N_{\downarrow} + N_d)!}$$

We briefly remember what we are currently working on....

$$|\Phi_G\rangle = \sum_{N_d} |\Phi(N_d)\rangle$$
  
$$\langle \Phi_G |\Phi_G\rangle = \sum_{N_d} \langle \Phi(N_d) |\Phi(N_d)\rangle$$

Question: which  $N_d$  gives the largest contribution  $W(N_d) = \langle \Phi(N_d) | \Phi(N_d) \rangle$  to this sum?

We just found

$$W(N_d) = \frac{N_{\uparrow}! \ N_{\downarrow}!}{N^{N_{\uparrow}+N_{\downarrow}}} (1-\lambda)^{2N_d} \frac{N!}{N_d! \ (N_{\uparrow}-N_d)! \ (N_{\downarrow}-N_d)! \ (N-N_{\uparrow}-N_{\downarrow}+N_d)!}$$

Take  $\log(W(N_d))$ , use Stirling formula for the factorials ...

 $\log(N!) \approx N \log(N) - N$ 

$$\frac{d\log(N!)}{dN} \approx \log(N) = \frac{\log((N+1)!) - \log(N!)}{1}$$

...and differentiate with respect to  $N_d$ :

$$\frac{d}{dN_d} \log (W(N_d)) = \log \left( (1-\lambda)^2 \frac{(N_{\uparrow} - N_d) (N_{\downarrow} - N_d)}{N_d (N - N_{\uparrow} - N_{\downarrow} + N_d)} \right)$$
$$\frac{d^2}{dN_d^2} \log (W(N_d)) = -\left( \frac{1}{N_d} + \frac{1}{N_{\uparrow} - N_d} + \frac{1}{N_{\downarrow} - N_d} + \frac{1}{N - N_{\uparrow} - N_{\downarrow} + N_d} \right)$$

We had

$$\frac{d}{dN_d} \log (W(N_d)) = \log \left( (1-\lambda)^2 \frac{(N_{\uparrow} - N_d) (N_{\downarrow} - N_d)}{N_d (N - N_{\uparrow} - N_{\downarrow} + N_d)} \right)$$
$$\frac{d^2}{dN_d^2} \log (W(N_d)) = -\left( \frac{1}{N_d} + \frac{1}{N_{\uparrow} - N_d} + \frac{1}{N_{\downarrow} - N_d} + \frac{1}{N - N_{\uparrow} - N_{\downarrow} + N_d} \right)$$

Switch to densities  $n_{\alpha} = N_{\alpha}/N$ ,  $\alpha \in \{\uparrow, \downarrow, d\}$ 

$$\frac{d}{dN_d} \log (W(N_d)) = \log \left( (1-\lambda)^2 \frac{(n_{\uparrow} - n_d) (n_{\downarrow} - n_d)}{n_d (1 - n_{\uparrow} - n_{\downarrow} + n_d)} \right)$$
  
$$\frac{d^2}{dN_d^2} \log (W(N_d)) = -\frac{1}{N} \left( \frac{1}{n_d} + \frac{1}{n_{\uparrow} - n_d} + \frac{1}{n_{\downarrow} - n_d} + \frac{1}{1 - n_{\uparrow} - n_{\downarrow} + n_d} \right)$$

Demanding  $\frac{d}{dN_d} \log (W(N_d)) = 0$  the first equation gives  $n_d(\lambda)$  (remember:  $n_{\uparrow}, n_{\downarrow}$  are given!)

$$(1-\lambda)^2 \frac{(n_{\uparrow} - n_d) (n_{\downarrow} - n_d)}{n_d (1 - n_{\uparrow} - n_{\downarrow} + n_d)} = 1$$

We had

$$(1-\lambda)^2 \, \frac{(n_\uparrow - n_d) \, (n_\downarrow - n_d)}{n_d \, (1-n_\uparrow - n_\downarrow + n_d)} \; = \; 1$$

For general  $n_{\sigma}$  this is involved - so put  $n_{\uparrow} = n_{\downarrow} = \frac{1}{2}$  (half-filling!):

$$(1-\lambda)^2 \frac{(\frac{1}{2}-n_d)^2}{n_d^2} = 1 \rightarrow n_d = \frac{1-\lambda}{2(2-\lambda)}$$

Check:  $\lambda \to 0$  - i.e. no projection - implies  $n_d = 1/4 = n_{\uparrow} \cdot n_{\downarrow}$  - correct at half-filling!

We have found the value  $N_{d,max}$  which gives the largest weight - the second derivative was

$$\frac{d^2}{dN_d^2} \log \left( W(N_d) \right) = -\frac{1}{N} \left( \frac{1}{n_d} + \frac{1}{n_{\uparrow} - n_d} + \frac{1}{n_{\downarrow} - n_d} + \frac{1}{1 - n_{\uparrow} - n_{\downarrow} + n_d} \right) = -\frac{c}{N}$$

All densities  $n_{\alpha}$  are of order unity  $\Rightarrow c$  is of order unity

Taylor expansion of the logarithm around  $N_{d,max}$  (remember:  $n_d = N_d/N \rightarrow N_d = N \cdot n_d$ )

$$\log(W(N_d)) = \log(W(N_{d,max})) - \frac{1}{2} \frac{c}{N} (N_d - N_{d,max})^2 + \dots$$

$$\Rightarrow W(N_d) = W(N_{d,max}) \cdot \exp\left(-\frac{c}{2N}(N_d - N_{d,max})^2\right) = W(N_{d,max}) \cdot \exp\left(-\frac{c}{2N}(n_d - n_{d,max})^2\right)$$

 $\rightarrow W(n_d)$  is a Gaussian of width  $\sqrt{\frac{2}{cN}} \Rightarrow$  as  $N \rightarrow \infty$  the width becomes zero

The Gutzwiller wave function consists of configurations with  $N_d = N \cdot n_{d,max}!$ 

The probability distribution for the number of double occupancies in the Gutzwiller wave function is a Gaussian with a width  $\propto \frac{1}{\sqrt{N}}$  and the center of the Gaussian is shifted by varying  $\lambda$ 



The expectation value of  $H_U$  therefore is trivial:  $\langle H_U \rangle = U \cdot N_d = U \cdot N \cdot n_d$ 

Expectation value of the kinetic energy

Basic idea: Reducing the number of double occupancies reduces the number of 'hopping possibilities'



#### The Gutzwiller Approximation

Basic assumption: the expectation value of the kinetic energy can be obtained from that of free electrons by multiplying by suitable renormalization factors  $\eta_{\sigma}$  which account for the reduced probability for hopping

$$\frac{\langle \Phi_G | H_t | \Phi_G \rangle}{\langle \Phi_G | \Phi_G \rangle} = \sum_{\sigma} \eta_{\sigma}(n_{\uparrow}, n_{\downarrow}, n_d) \langle FS, \sigma | H_t | FS, \sigma \rangle$$

 $|FS, \sigma\rangle$ : Fermi sea for  $\sigma$ -electrons

 $\eta_{\sigma}(n_{\uparrow}, n_{\downarrow}, n_{d}) = \frac{Number \ of \ hopping \ possibilities \ with \ n_{d} \ double \ occupancies}{Number \ of \ hopping \ possibilities \ with \ n_{d} = n_{\uparrow} \cdot n_{\downarrow}}$ 

The evaluation of the  $\eta_{\sigma}(n_{\uparrow}, n_{\downarrow}, n_d)$  then is a combinatorical problem - this is discussed very understandably by Ogawa *et al.* Progr. Theor. Phys. **53**, 614 (1975).

Introduce fictitious Hilbert space with 4 'book-keeping kets' for every site  $i: |i, 0\rangle$ ,  $|i, \uparrow\rangle$ ,  $|i, \downarrow\rangle$  and  $|i, \uparrow\downarrow\rangle$ 

Define a wave function of a single site i (with  $\alpha_{\sigma}$ ,  $\beta$  real).....

$$|B_i\rangle = \frac{|i,0\rangle + \alpha_{\uparrow} |i,\uparrow\rangle + \alpha_{\downarrow} |i,\downarrow\rangle + \beta |i,\uparrow\downarrow\rangle}{\sqrt{1 + \alpha_{\uparrow}^2 + \alpha_{\downarrow}^2 + \beta^2}}$$
$$\langle B_i| B_i\rangle = 1$$

... and a wave function of the whole lattice

$$|\Psi\rangle = \prod_{i} |B_{i}\rangle$$
$$\langle \Psi|\Psi\rangle = 1$$

We had

$$|B_i\rangle = \frac{|i,0\rangle + \alpha_{\uparrow} |i,\uparrow\rangle + \alpha_{\downarrow} |i,\downarrow\rangle + \beta |i,\uparrow\downarrow\rangle}{\sqrt{1 + \alpha_{\uparrow}^2 + \alpha_{\downarrow}^2 + \beta^2}}$$
$$|\Psi\rangle = \prod_i |B_i\rangle$$

If  $|\Psi\rangle$  were a true electron state we would have

$$\langle N_{\uparrow} \rangle = N \frac{\alpha_{\uparrow}^2 + \beta^2}{1 + \alpha_{\uparrow}^2 + \alpha_{\downarrow}^2 + \beta^2}, \\ \langle N_d \rangle = N \frac{\beta^2}{1 + \alpha_{\uparrow}^2 + \alpha_{\downarrow}^2 + \beta^2}.$$

which can be reverted to give

$$\alpha_{\sigma} = \sqrt{\frac{n_{\sigma} - n_d}{1 - n_{\uparrow} - n_{\downarrow} + n_d}},$$
  
$$\beta = \sqrt{\frac{n_d}{1 - n_{\uparrow} - n_{\downarrow} + n_d}}.$$

Our auxilliary wave function was (remember:  $(\alpha_{\uparrow}, \alpha_{\downarrow}, \beta) \leftrightarrow (n_{\uparrow}, n_{\downarrow}, n_d))$ 

$$|B_i\rangle = \frac{|i,0\rangle + \alpha_{\uparrow}|i,\uparrow\rangle + \alpha_{\downarrow}|i,\downarrow\rangle + \beta|i,\uparrow\downarrow\rangle}{\sqrt{1 + \alpha_{\uparrow}^2 + \alpha_{\downarrow}^2 + \beta^2}}$$
$$|\Psi\rangle = \prod_i |B_i\rangle$$

 $|\Psi\rangle$  has norm 1 and as many 'empty sites', 'singly occupied sites' and 'doubly occupied sites' as the true Gutzwiller wave function if we adjust  $\alpha_{\sigma}$  and  $\beta$  correctly

But:  $|\Psi\rangle$  does not correspond to a state with fixed electron number  $\Rightarrow$  in principle we should instead use

$$|\Psi'\rangle = \mathcal{P}(N_{\uparrow}, N_{\downarrow}, N_{d}) |\Psi\rangle$$

where  $\mathcal{P}$  projects onto the component of  $|\Psi\rangle$  which has precisely  $\langle N_{\uparrow}\rangle$   $\uparrow$ -electrons etc.

But<sup>2</sup>: It is straightforward to show that the probability distribution of the  $N_{\alpha}$  - with  $\alpha \in \{\uparrow, \downarrow, d\}$  have a Gaussian distribution around their mean values  $\bar{N}_{\alpha}$  with a width which is again  $\propto N^{-1/2}$ 

Therefore, in calculating expectation values we may drop the projector  ${\cal P}$  and replace  $|\Psi'
angle o |\Psi
angle$ 

Compare J. Bardeen, L. N. Cooper, and J. R. Schrieffer Phys. Rev. 106, 162 (1957)

$$|\Psi_{BCS}\rangle = \mathcal{P} \prod_{\boldsymbol{k}} \left( u_{\boldsymbol{k}} + v_{\boldsymbol{k}} c^{\dagger}_{\boldsymbol{k},\uparrow} c^{\dagger}_{-\boldsymbol{k},\downarrow} \right) |0\rangle$$

 $\text{Our auxilliary wave function was (remember: } (\alpha_{\uparrow}, \alpha_{\downarrow}, \beta) \leftrightarrow (n_{\uparrow}, n_{\downarrow}, n_d) \textbf{)}$ 

$$|B_i\rangle = \frac{|i,0\rangle + \alpha_{\uparrow}|i,\uparrow\rangle + \alpha_{\downarrow}|i,\downarrow\rangle + \beta|i,\uparrow\downarrow\rangle}{\sqrt{1 + \alpha_{\uparrow}^2 + \alpha_{\downarrow}^2 + \beta^2}}$$
$$|\Psi\rangle = \prod_i |B_i\rangle$$

Now we 'translate' the electron operators (note: this ignores the Fermi sign)

$$\tilde{c}_{i,\uparrow} = |i,0\rangle \langle i,\uparrow | + |i,\downarrow\rangle \langle i,\uparrow\downarrow |$$

Then we estimate the number of hopping possibilities per bond as

$$h(\uparrow, n_{\uparrow}, n_{\downarrow}, n_{d}) = \frac{\langle \Psi | \tilde{c}_{i,\uparrow}^{\dagger} \, \tilde{c}_{j,\uparrow} | \Psi \rangle}{\langle \Psi | \Psi \rangle} = \langle \Psi | \tilde{c}_{i,\uparrow}^{\dagger} \, \tilde{c}_{j,\uparrow} | \Psi \rangle = \langle B_{i} | \tilde{c}_{i,\uparrow}^{\dagger} | B_{i} \rangle \, \langle B_{j} | \tilde{c}_{j,\uparrow} | B_{j} \rangle$$
$$= |\langle B_{i} | \tilde{c}_{i,\uparrow} | B_{i} \rangle|^{2} = \left( \frac{\alpha_{\uparrow} + \alpha_{\downarrow} \beta}{1 + \alpha_{\uparrow}^{2} + \alpha_{\downarrow}^{2} + \beta^{2}} \right)^{2}$$

Number of hopping possibilities per bond  $h(\sigma, n_{\uparrow}, n_{\downarrow}, n_d) = \left(\frac{\alpha_{\sigma} + \alpha_{-\sigma}\beta}{1 + \alpha_{\uparrow}^2 + \alpha_{\downarrow}^2 + \beta^2}\right)^2$ 

We found earlier how  $\alpha_{\sigma}$  and  $\beta$  can be expressed by  $n_{\sigma}$  and  $n_{d}$ ....

$$\alpha_{\sigma} = \sqrt{\frac{n_{\sigma} - n_d}{1 - n_{\uparrow} - n_{\downarrow} + n_d}}, \qquad \beta = \sqrt{\frac{n_d}{1 - n_{\uparrow} - n_{\downarrow} + n_d}}.$$

.... and inserting this we find

$$h(\sigma, n_{\uparrow}, n_{\downarrow}, n_d) = \left(\sqrt{n_{\sigma} - n_d} \sqrt{1 - n_{\uparrow} - n_{\downarrow} + n_d} + \sqrt{n_d} \sqrt{n_{-\sigma} - n_d}\right)^2$$

The final renormalization factor then is obtained by dividing

$$\eta(\sigma, n_{\uparrow}, n_{\downarrow}, n_{d}) = \frac{h(\sigma, n_{\uparrow}, n_{\downarrow}, \mathbf{n}_{d})}{h(\sigma, n_{\uparrow}, n_{\downarrow}, \mathbf{n}_{\uparrow} \mathbf{n}_{\downarrow})} = \left(\frac{\sqrt{n_{\sigma} - n_{d}}\sqrt{1 - n_{\uparrow} - n_{\downarrow} + n_{d}} + \sqrt{n_{d}}\sqrt{n_{-\sigma} - n_{d}}}{\sqrt{n_{\sigma}(1 - n_{\sigma})}}\right)^{2}$$

## Collecting everything

We decomposed the Gutzwiller wave function into components with fixed number of double occupancies

$$|\Phi_G\rangle = \sum_{N_d} |\Phi(N_d)\rangle$$

 $\langle \Phi(N_d) | \Phi(N_d) \rangle$  is the probability distribution for the number of double occupancies and we found this is 'infinitely sharply peaked' around  $N_d = N \cdot n_d$  with

$$(1-\lambda)^2 \frac{(n_{\uparrow} - n_d) (n_{\downarrow} - n_d)}{n_d (1 - n_{\uparrow} - n_{\downarrow} + n_d)} = 1$$

This equation allows to switch from  $\lambda \rightarrow n_d$  as variational parameter!

The expectation value of  $H_U$  then becomes trivial

$$\langle H_U \rangle = N \cdot U \cdot n_d$$

The expectation value of the kinetic energy was approximated as

$$\langle H_t \rangle = \sum_{\sigma} \eta(\sigma, n_{\uparrow}, n_{\downarrow}, n_d) \langle FS, \sigma | H_t | FS, \sigma \rangle$$

with the renormalization factors  $\eta_\sigma$ 

 $\eta_{\sigma}(n_{\uparrow}, n_{\downarrow}, n_{d}) = \frac{Number \ of \ hopping \ possibilities \ with \ n_{d} \ double \ occupancies}{Number \ of \ hopping \ possibilities \ with \ n_{d} = n_{\uparrow} \cdot n_{\downarrow}}$ 

Their evaluation is a combinatorical problem and they can be expressed as functions of  $n_{\uparrow}$ ,  $n_{\downarrow}$  and  $n_d$ 

$$\eta(\sigma, n_{\uparrow}, n_{\downarrow}, n_d) = \left(\frac{\sqrt{n_{\sigma} - n_d}\sqrt{1 - n_{\uparrow} - n_{\downarrow} + n_d} + \sqrt{n_d}\sqrt{n_{-\sigma} - n_d}}{\sqrt{n_{\sigma}(1 - n_{\sigma})}}\right)^2$$

We thus have calculated the expectation value of the energy as a function of  $n_d$ 

Here it is:

$$E = \langle H_t \rangle + \langle H_U \rangle = \sum_{\sigma} \eta_{\sigma}(\sigma, n_{\uparrow}, n_{\downarrow}, n_d) \langle FS, \sigma | H_t | FS, \sigma \rangle + N \cdot U \cdot n_d$$

We specialize to the nonmagnetic case  $n_{\uparrow}=n_{\downarrow}$  and divide by N (i.e. we consider the energy per site)

$$e = \eta(n_{\sigma}, n_d) \, \frac{\mathbf{t}_0}{\mathbf{t}_0} + U \, n_d$$

where  $t_0$  is the kinetic energy of the Fermi sea per site - which can be obtained by numerical integration

$$t_0 = \frac{2}{N} \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} \Theta(E_F - \epsilon_{\mathbf{k}})$$

We further specialize to  $n_{\sigma} = \frac{1}{2}$ 

$$\eta(n_d) = 16 \ n_d \ (\frac{1}{2} - n_d)$$
$$e(n_d) = 16 \ n_d \ (\frac{1}{2} - n_d) \ t_0 + U \ n_d$$

Demanding  $\frac{de}{dn_d} = 0$  we find the  $n_d$  (or  $\lambda$ ) which minimizes the energy

$$n_d = \frac{1}{4} - \frac{U}{32|t_0|}$$

The  $n_d$  which minimizes the energy was

$$n_d = \frac{1}{4} - \frac{U}{32|t_0|}$$

This decreases linearly with U and becomes zero for

$$U_c = 8|t_0|$$

This is the famous Brinkman-Rice transition

For the 2D square lattice with nearest neigbor hopping we obtain  $t_0 = -1.621 t \Rightarrow U_c = 12.969 t$
The Gutzwiller wave function was

$$|\Phi_G\rangle = \prod_i (1 - \lambda \ n_{i,\uparrow} n_{i,\downarrow}) \ |FS\rangle,$$

The wave function for a state with a hole-like quasiparticle then would be

$$|\Phi_G(\mathbf{k})\rangle = \prod_i (1 - \lambda' n_{i,\uparrow} n_{i,\downarrow}) c_{\mathbf{k},\uparrow} |FS\rangle,$$

The 'quasiparticle dispersion' then can be obtained from

$$\tilde{\epsilon}_{\mathbf{k}} = \frac{\langle \Phi_G | H | \Phi_G \rangle}{\langle \Phi_G | \Phi_G \rangle} - \frac{\langle \Phi_G (\mathbf{k}) | H | \Phi_G (\mathbf{k}) \rangle}{\langle \Phi_G (\mathbf{k}) | \Phi_G (\mathbf{k}) \rangle}$$

$$|\Phi_G(\mathbf{k})\rangle = \prod_i (1 - \lambda' n_{i,\uparrow} n_{i,\downarrow}) c_{\mathbf{k},\uparrow} |FS\rangle,$$

The condition on  $n_d$  (i.e.  $\lambda'$ ) was the minimization of the energy per site

$$e = \eta(n_{\sigma}, n_d) t_0 + n_d U \Rightarrow 0 = \frac{\partial \eta}{\partial n_d} t_0 + U$$

The variational procedure for  $|\Phi_G({f k})
angle$  amounts to

$$e \rightarrow e - \frac{1}{N} \tilde{\epsilon}_{\mathbf{k}}$$
$$t_0 \rightarrow t_0 - \frac{1}{N} \epsilon_{\mathbf{k}}$$
$$n_{\uparrow} \rightarrow n_{\uparrow} - \frac{1}{N}$$
$$n_d \rightarrow n_d + \frac{1}{N} \delta n_d$$

Inserting and expanding gives

$$\boldsymbol{e} - \frac{1}{N} \, \tilde{\epsilon_{\mathbf{k}}} = \left( \eta(\boldsymbol{n_{\sigma}}, \boldsymbol{n_{d}}) - \frac{1}{N} \, \frac{\partial \eta}{\partial \boldsymbol{n_{\uparrow}}} + \frac{1}{N} \, \frac{\partial \eta}{\partial \boldsymbol{n_{d}}} \, \delta \boldsymbol{n_{d}} \right) \left( \boldsymbol{t_{0}} - \frac{1}{N} \, \boldsymbol{\epsilon_{\mathbf{k}}} \right) + \boldsymbol{n_{d}} \, \boldsymbol{U} + \frac{1}{N} \, \delta \boldsymbol{n_{d}} \, \boldsymbol{U}$$

$$|\Phi_G(\mathbf{k})\rangle = \prod_i (1 - \lambda' n_{i,\uparrow} n_{i,\downarrow}) c_{\mathbf{k},\uparrow} |FS\rangle,$$

The condition on  $n_d$  (i.e.  $\lambda'$ ) was the minimization of the energy per site

$$e = \eta(n_{\sigma}, n_d) t_0 + n_d U \Rightarrow 0 = \frac{\partial \eta}{\partial n_d} t_0 + U$$

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$$e \rightarrow e - \frac{1}{N} \tilde{\epsilon}_{\mathbf{k}}$$
$$t_0 \rightarrow t_0 - \frac{1}{N} \epsilon_{\mathbf{k}}$$
$$n_{\uparrow} \rightarrow n_{\uparrow} - \frac{1}{N}$$
$$n_d \rightarrow n_d + \frac{1}{N} \delta n_d$$

Inserting and expanding gives

$$\tilde{\epsilon_{\mathbf{k}}} = \eta(n_{\sigma}, n_d) \, \epsilon_{\mathbf{k}} + t_0 \, \frac{1}{2} \left( \frac{\partial \eta_{\uparrow}}{\partial n_{\uparrow}} + \frac{\partial \eta_{\downarrow}}{\partial n_{\uparrow}} \right) - \delta n_d \, \left( \frac{\partial \eta}{\partial n_d} \, t_0 + U \right)$$

$$\tilde{\epsilon_{\mathbf{k}}} = \eta(n_{\sigma}, n_d) \ \epsilon_{\mathbf{k}} + t_0 \ \frac{1}{2} \left( \frac{\partial \eta_{\uparrow}}{\partial n_{\uparrow}} + \frac{\partial \eta_{\downarrow}}{\partial n_{\uparrow}} \right) = \eta(n_{\sigma}, n_d) \ \epsilon_{\mathbf{k}} + C$$

The quasiparticle dispersion is renormalized by the same factor  $\eta$  as the expectation value of the kinetic energy (C can be absorbed in a shift of  $\mu$ )



At the Brinkman-Rice transition (for half-filling) we had  $\eta \to 0$ 

The Gutzwiller wave function describes the metal insulator transition at half-filling by the vanishing of the bandwidth or, alternatively, by the divergence of the effective mass

Suppose we choose  $U > U_c$  (Brinkman-Rice!) so that the system is a Mott-insulator at half-filling

What happens in the lightly doped Mott-insulator i.e we start from the doped case  $n_e < 1$  and let  $n_e \rightarrow 1$ ?

The condition on  $n_d$  continues to be minimization of the GS-energy per site...

$$e = \eta(n_{\sigma}, n_d) t_0 + n_d U$$

... but this now has to be done numerically - the result is (2D square lattice,  $U/t = 16 > U_c/t = 12.969$ )



## Summary, Gutzwiller Wave Function

- Basis idea: gound state corresponds to a 'Fermi sea' with the same number of quasiparticles as the free electrons system, but reduced band width (and kinetic energy)
- This correlation narrowing takes into account that electrons have fewer possibilities to hop due to a reduction of the number of double occupancies
- The Fermi surface agrees with the free electron Fermi surface
- The metal-insulator transition (Brinkman-Rice transition) is realized by a vanishing bandwidth divergence of the effective mass

We consider the case of large U/t such that the system is a Mott-insulator at half-filling,  $n_e = 1$ How does the system behave as  $n_e \rightarrow 1$  from below?

Hubbard-I approximation and Gutzwiller wave function describe two completely different scenarios



(From W. J. Padilla *et al.*, PRB 72,060511 (2005): Hall constant and Drude weight as functions of  $1 - n_e$ )



Dissipative part of optical conductivity in Drude theory:

$$\sigma_1(\omega) = \frac{ne^2}{m^*} \frac{\tau^{-1}}{\omega^2 + \tau^{-2}}$$

( $\tau^{-1}$ : inverse lifetime, n: carrier density,  $m^*$ : 'optical mass') It follows that

$$N_{eff} = \int_0^\infty \ d\omega \ \sigma_1(\omega) = \frac{ne^2}{m^*} \ \frac{\pi}{2}$$

In practice the integral is carried out only up to  $\omega_{max} = 650 \ cm^{-1}$  so as to pick up only the Drude peak The Hall constant is in Drude theory:

$$R_H = \frac{1}{ne}$$

we have

$$m^* = \frac{1}{R_H N_{eff}} \frac{2}{e\pi}$$

(From W. J. Padilla *et al.*, PRB 72,060511 (2005): Hall constant and Drude weight as functions of  $1 - n_e$ )



## Summary

Which 'true' behaviour might the Hubbard-I approximation be 'trying to approximate'?



Perhaps a phase transition between two phases of different Fermi surface volume?

Does one see anything like this in experiment?



Underdoped cuprate superconductors show 'Fermi arcs' ( $x = 1 - n_e$ )



ARPES spectra on  $La_{2-x}Sr_xCuO_4$  (20 K) from T. Yoshida *et al.*, J. Phys. Soc. Jpn. 81 011006 (2012).

These may also be 'half of a pocket'



T-dependence of resitivity in HgBa<sub>2</sub>CoO<sub>4+ $\delta$ </sub>: (Barisic et al., Proc. Nat. Acad. Sci. 110, 12235 (2013))



 $\rho(T) = A_1 T \qquad T > 280 K$  $\rho(T) = A_2 T^2 \qquad T < 170 K$ 

The prefactors  $A_1$  and  $A_2$  vary with hole concentration  $\delta = 1 - n_e$  Doping dependence of prefactors:  $A_1$ ,  $A_2 \propto \frac{1}{\delta}$ 



We had  $\rho(T) = A_1 T$  and  $\rho(T) = A_2 T^2$  and in both cases  $A \propto \frac{1}{\delta}$  - this can be explained like this

$$\sigma = \frac{ne^2\tau}{m^*} \quad \rightarrow \quad \rho = \frac{m^*}{ne^2\tau} = \frac{m^*/e^2}{n} \tau^{-1}$$

with inverse lifetime  $\tau^{-1} \propto T, T^2$  and carrier density  $n = \delta \rightarrow$  Fermi surface volume  $\propto \delta$ (we have seen before that  $m^*$  is doping independent)



Transport properties also are consistent with a 'small' Fermi surface

(Data from W. J. Padilla *et al.*, PRB **72**,060511 (2005) - remember:  $n_e = 1 - x$ )

## Therefore



Possible Scenario

Question: Which 'true' behaviour might the Hubbard-I approximation be 'trying to approximate'?



Perhaps a phase transition between two phases of different Fermi surface volume?

• The interaction term  $H_U = U n_{i,\uparrow} n_{i,\downarrow}$  can be rewritten:

- The system can lower its energy by forming magnetic moments:  $\langle S_i^2 \rangle \neq 0$
- The moments can be static  $\langle S_i \rangle \neq 0$  or fluctuating  $\langle S_i \rangle = 0$
- The Hubbard dimer was an example for fluctuating moments
- Spin density wave theory deals with static moments

- We consider a 2D square lattice with N sites with a static moment  $\langle S_i \rangle \neq 0$  at each site
- From the solution of the Hubbard dimer we know that the spins on sites connected by the hopping term prefer to be antiparallel
- If we assume hopping only between nearest neighbors this defines the Néel state:

↓	₹	↓	₹	
₹	↓	ŧ	↓	
↓	ŧ	↓	ŧ	
<b>≜</b>	↓	ŧ	↓	

• Accordingly we set (with  $Q = (\frac{\pi}{a}, \frac{\pi}{a})$ , a lattice constant)

$$\langle n_{i,\uparrow} \rangle = \frac{n_e}{2} + \frac{m}{2} e^{i \mathbf{Q} \cdot \mathbf{R}_i}, \qquad \langle n_{i,\downarrow} \rangle = \frac{n_e}{2} - \frac{m}{2} e^{i \mathbf{Q} \cdot \mathbf{R}_i},$$

$$\Rightarrow \langle n_i \rangle = \langle n_{i,\uparrow} \rangle + \langle n_{i,\downarrow} \rangle = n_e, \qquad \langle S_i^z \rangle = \frac{1}{2} \left( \langle n_{i,\uparrow} \rangle - \langle n_{i,\downarrow} \rangle \right) = \frac{m}{2} e^{i\mathbf{Q} \cdot \mathbf{R}_i}.$$

Let  $\mathbf{R}_i = (ma, na) \Rightarrow e^{i\mathbf{Q}\cdot\mathbf{R}_i} = e^{i(m+n)\pi}$  which is +1 (-1) if (m+n) is even (odd)

We set

$$n_{i,\sigma} = \langle n_{i,\sigma} \rangle + \delta n_{i,\sigma}$$
  $\delta n_{i,\sigma} = n_{i,\sigma} - \langle n_{i,\sigma} \rangle$ 

- $\delta n_{i,\sigma}$  is the operator of fluctuations of  $n_{i,\sigma}$  around its mean value  $\langle n_{i,\sigma} \rangle$
- We assume that fluctuations are 'small' this is the basic assumption of any mean-field theory
- Then we can approximate the interaction term

$$U n_{i,\uparrow} n_{i,\downarrow} = U(\langle n_{i,\uparrow} \rangle + \delta n_{i,\uparrow})(\langle n_{i,\downarrow} \rangle + \delta n_{i,\downarrow})$$
  
=  $U (\langle n_{i,\uparrow} \rangle \langle n_{i,\downarrow} \rangle + \langle n_{i,\uparrow} \rangle \delta n_{i,\downarrow} + \langle n_{i,\downarrow} \rangle \delta n_{i,\uparrow} + \delta n_{i,\uparrow} \delta n_{i,\downarrow})$   
 $\approx U (\langle n_{i,\uparrow} \rangle n_{i,\downarrow} + \langle n_{i,\downarrow} \rangle n_{i,\uparrow} - \langle n_{i,\uparrow} \rangle \langle n_{i,\downarrow} \rangle)$ 

Now insert 
$$\langle n_{i,\uparrow} \rangle = \frac{n_e}{2} + \frac{m}{2} e^{i \mathbf{Q} \cdot \mathbf{R}_i}$$
  $\langle n_{i,\downarrow} \rangle = \frac{n_e}{2} - \frac{m}{2} e^{i \mathbf{Q} \cdot \mathbf{R}_i}$ 

and find  $U n_{i,\uparrow} n_{i,\downarrow} \approx \frac{n_e U}{2} \sum_{\sigma} n_{i,\sigma} - \frac{mU}{2} e^{i \mathbf{Q} \cdot \mathbf{R}_i} (n_{i,\uparrow} - n_{i,\downarrow}) - U \frac{n_e^2 - m^2}{4}$ 

This is now quadratic in c-operators so and thus H can be diagonalized by unitary transformation!

$$U n_{i,\uparrow} n_{i,\downarrow} = \frac{n_e U}{2} \sum_{\sigma} n_{i,\sigma} - \frac{mU}{2} e^{i \mathbf{Q} \cdot \mathbf{R}_i} (n_{i,\uparrow} - n_{i,\downarrow}) - U \frac{n_e^2 - m^2}{4}$$

Now switch to Fourier transformed *c*-operators and add the kinetic energy

$$H_0 = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma}$$

- the mean-field Hamiltonian  $K = H - \mu N$  then becomes

$$K_{MF} = \sum_{\mathbf{k},\sigma} \tilde{\epsilon}_{\mathbf{k}} c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} - \Delta \sum_{\mathbf{k}} \left( c^{\dagger}_{\mathbf{k},\uparrow} c_{\mathbf{k}+\mathbf{Q},\uparrow} - c^{\dagger}_{\mathbf{k},\downarrow} c_{\mathbf{k}+\mathbf{Q},\downarrow} \right) - NU \frac{n_e^2 - m^2}{4}$$

whereby

$$\tilde{\epsilon}_{\mathbf{k}} = \epsilon_{\mathbf{k}} + \frac{n_e U}{2} - \mu \qquad \qquad \Delta = \frac{mU}{2}$$

$$K_{MF} = \sum_{\mathbf{k},\sigma} \tilde{\epsilon}_{\mathbf{k}} c_{\mathbf{k},\sigma}^{\dagger} c_{\mathbf{k},\sigma} - \Delta \sum_{\mathbf{k}} \left( c_{\mathbf{k},\uparrow}^{\dagger} c_{\mathbf{k}+\mathbf{Q},\uparrow} - c_{\mathbf{k},\downarrow}^{\dagger} c_{\mathbf{k}+\mathbf{Q},\downarrow} \right) - NU \frac{n_e^2 - m^2}{4},$$

Now we follow Gorkov (Soviet Phys. JETP 7, 505 (1958)), and define the imaginary-time Green's function

$$G_{\sigma}(\mathbf{k},\tau) = -\langle T c_{\mathbf{k},\sigma}(\tau) c_{\mathbf{k},\sigma}^{\dagger} \rangle = -\Theta(\tau) \langle c_{\mathbf{k},\sigma}(\tau) c_{\mathbf{k},\sigma}^{\dagger} \rangle + \Theta(-\tau) \langle c_{\mathbf{k},\sigma}^{\dagger} c_{\mathbf{k},\sigma}(\tau) \rangle$$

This obeys the equation of motion (upper sign for  $\sigma = \uparrow$ )

$$\begin{aligned} -\frac{\partial}{\partial \tau} G_{\sigma}(\mathbf{k},\tau) &= \delta(\tau) \left\langle \{c_{\mathbf{k},\sigma}^{\dagger}, c_{\mathbf{k},\sigma}\} \right\rangle - \left\langle T \left[ c_{\mathbf{k},\sigma}, K_{MF} \right](\tau) c_{\mathbf{k},\sigma}^{\dagger} \right\rangle \\ &= \delta(\tau) - \left\langle T \left( \tilde{\epsilon}_{\mathbf{k}} c_{\mathbf{k},\sigma}(\tau) \mp \Delta c_{\mathbf{k}+\mathbf{Q},\sigma}(\tau) \right) c_{\mathbf{k},\sigma}^{\dagger} \right\rangle \\ &= \delta(\tau) + \tilde{\epsilon}_{\mathbf{k}} \left( - \left\langle T c_{\mathbf{k},\sigma}(\tau) c_{\mathbf{k},\sigma}^{\dagger} \right\rangle \right) \mp \Delta \left( - \left\langle T c_{\mathbf{k}+\mathbf{Q},\sigma}(\tau) c_{\mathbf{k},\sigma}^{\dagger} \right\rangle \right) \\ &= \delta(\tau) + \tilde{\epsilon}_{\mathbf{k}} G_{\sigma}(\mathbf{k},\tau) \mp \Delta \tilde{G}_{\sigma}(\mathbf{k},\tau), \end{aligned}$$

with the anomalous Green's function  $\tilde{G}_{\sigma}(\mathbf{k},\tau) = -\langle T c_{\mathbf{k}+\mathbf{Q},\sigma}(\tau) c_{\mathbf{k},\sigma}^{\dagger} \rangle$ 

$$\begin{split} K_{MF} &= \sum_{\mathbf{k},\sigma} \tilde{\epsilon}_{\mathbf{k}} c_{\mathbf{k},\sigma}^{\dagger} c_{\mathbf{k},\sigma} - \Delta \sum_{\mathbf{k}} \left( c_{\mathbf{k},\uparrow}^{\dagger} c_{\mathbf{k}+\mathbf{Q},\uparrow} - c_{\mathbf{k},\downarrow}^{\dagger} c_{\mathbf{k}+\mathbf{Q},\downarrow} \right) - NU \, \frac{n_{e}^{2} - m^{2}}{4} \\ - \frac{\partial}{\partial \tau} G_{\sigma}(\mathbf{k},\tau) &= \delta(\tau) + \tilde{\epsilon}_{\mathbf{k}} \, G_{\sigma}(\mathbf{k},\tau) \mp \Delta \, \tilde{G}_{\sigma}(\mathbf{k},\tau), \\ \tilde{G}_{\sigma}(\mathbf{k},\tau) &= -\langle T \, c_{\mathbf{k}+\mathbf{Q},\sigma}(\tau) \, c_{\mathbf{k},\sigma}^{\dagger} \rangle \end{split}$$

Proceeding as above we find the second equation of motion

$$\Rightarrow -\frac{\partial}{\partial \tau} \tilde{G}_{\sigma}(\mathbf{k},\tau) = \tilde{\epsilon}_{\mathbf{k}+\mathbf{Q}} \tilde{G}_{\sigma}(\mathbf{k},\tau) \mp \Delta G_{\sigma}(\mathbf{k},\tau).$$

The system of equations of motion closes:

$$-\frac{\partial}{\partial \tau} G_{\sigma}(\mathbf{k},\tau) - \tilde{\epsilon}_{\mathbf{k}} \quad G_{\sigma}(\mathbf{k},\tau) \pm \Delta \tilde{G}_{\sigma}(\mathbf{k},\tau) = \delta(\tau)$$
$$-\frac{\partial}{\partial \tau} \tilde{G}_{\sigma}(\mathbf{k},\tau) - \tilde{\epsilon}_{\mathbf{k}+\mathbf{Q}} \tilde{G}_{\sigma}(\mathbf{k},\tau) \pm \Delta G_{\sigma}(\mathbf{k},\tau) = 0$$

$$-\frac{\partial}{\partial \tau} G_{\sigma}(\mathbf{k},\tau) - \tilde{\epsilon}_{\mathbf{k}} \quad G_{\sigma}(\mathbf{k},\tau) \pm \Delta \tilde{G}_{\sigma}(\mathbf{k},\tau) = \delta(\tau) \\ -\frac{\partial}{\partial \tau} \tilde{G}_{\sigma}(\mathbf{k},\tau) - \tilde{\epsilon}_{\mathbf{k}+\mathbf{Q}} \tilde{G}_{\sigma}(\mathbf{k},\tau) \pm \Delta G_{\sigma}(\mathbf{k},\tau) = 0$$

After Fourier transformation with respect to  $\boldsymbol{\tau}$ 

$$G_{\sigma}(\mathbf{k},\tau) = \frac{1}{\beta} \sum_{\nu = -\infty}^{\infty} e^{-i\omega_{\nu}\tau} G_{\sigma}(\mathbf{k},i\omega_{\nu}) \qquad \qquad \delta(\tau) = \frac{1}{\beta} \sum_{\nu = -\infty}^{\infty} e^{-i\omega_{\nu}\tau}$$

so that  $-\partial_{\tau} \rightarrow i\omega_{\nu}$ :

$$(i\omega_{\nu} - \tilde{\epsilon}_{\mathbf{k}}) G_{\sigma}(\mathbf{k}, i\omega_{\nu}) \pm \Delta \tilde{G}_{\sigma}(\mathbf{k}, i\omega_{\nu}) = 1$$
$$(i\omega_{\nu} - \tilde{\epsilon}_{\mathbf{k}+\mathbf{Q}}) \tilde{G}_{\sigma}(\mathbf{k}, i\omega_{\nu}) \pm \Delta G_{\sigma}(\mathbf{k}, i\omega_{\nu}) = 0$$

This can be written in matrix form

$$\begin{pmatrix} i\omega_{\nu} - \tilde{\epsilon}_{\mathbf{k}} & \pm\Delta \\ \pm\Delta & i\omega_{\nu} - \tilde{\epsilon}_{\mathbf{k}+\mathbf{Q}} \end{pmatrix} \begin{pmatrix} G_{\sigma}(\mathbf{k}, i\omega_{\nu}) \\ \tilde{G}_{\sigma}(\mathbf{k}, i\omega_{\nu}) \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\begin{pmatrix} i\omega_{\nu} - \tilde{\epsilon}_{\mathbf{k}} & \pm\Delta \\ \pm\Delta & i\omega_{\nu} - \tilde{\epsilon}_{\mathbf{k}+\mathbf{Q}} \end{pmatrix} \begin{pmatrix} G_{\sigma}(\mathbf{k}, i\omega_{\nu}) \\ \tilde{G}_{\sigma}(\mathbf{k}, i\omega_{\nu}) \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

Now define

$$\begin{split} \zeta_{k} &= \frac{1}{2} \left( \tilde{\epsilon}_{k} + \tilde{\epsilon}_{k+Q} \right), & \eta_{k} &= \frac{1}{2} \left( \tilde{\epsilon}_{k} - \tilde{\epsilon}_{k+Q} \right), \\ \tilde{\epsilon}_{k} &= \zeta_{k} + \eta_{k} & \tilde{\epsilon}_{k+Q} &= \zeta_{k} - \eta_{k} \end{split}$$

so that

$$\begin{pmatrix} i\omega_{\nu} - \zeta_{\mathbf{k}} - \eta_{\mathbf{k}} & \pm \Delta \\ \pm \Delta & i\omega_{\nu} - \zeta_{\mathbf{k}} + \eta_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} G_{\sigma}(\mathbf{k}, i\omega_{\nu}) \\ \tilde{G}_{\sigma}(\mathbf{k}, i\omega_{\nu}) \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}.$$

$$\begin{pmatrix} i\omega_{\nu} - \zeta_{\mathbf{k}} - \eta_{\mathbf{k}} & \pm \Delta \\ \pm \Delta & i\omega_{\nu} - \zeta_{\mathbf{k}} + \eta_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} G_{\sigma}(\mathbf{k}, i\omega_{\nu}) \\ \tilde{G}_{\sigma}(\mathbf{k}, i\omega_{\nu}) \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}.$$

The matrix on the l.h.s. can be written as (with 1:  $2 \times 2$  unit matrix,  $\tau$ : Pauli matrices)

$$(i\omega_{
u}-\zeta_{k}) \mathbf{1} \pm \Delta \tau_{x} - \eta_{k} \tau_{z}$$

One can show (Landau-Lifshitz, Quantum Mechanics) that for any a and any vector b:

$$(a\mathbf{1} + \mathbf{b} \cdot \boldsymbol{\tau})(a\mathbf{1} - \mathbf{b} \cdot \boldsymbol{\tau}) = a^2 - \mathbf{b}^2 \qquad \Rightarrow \qquad (a\mathbf{1} + \mathbf{b} \cdot \boldsymbol{\tau})^{-1} = \frac{a\mathbf{1} - \mathbf{b} \cdot \boldsymbol{\tau}}{a^2 - \mathbf{b}^2}.$$

In our case  $a = i\omega_{\nu} - \zeta_k$ ,  $b = (\pm\Delta, 0, -\eta_k)$  Therefore

$$\begin{pmatrix} G_{\sigma}(\mathbf{k}, i\omega_{\nu}) \\ \tilde{G}_{\sigma}(\mathbf{k}, i\omega_{\nu}) \end{pmatrix} = \frac{1}{(i\omega_{\nu} - \zeta_{\mathbf{k}})^2 - (\Delta^2 + \eta_{\mathbf{k}}^2)} \begin{pmatrix} i\omega_{\nu} - \zeta_{\mathbf{k}} + \eta_{\mathbf{k}} & \mp \Delta \\ \mp \Delta & i\omega_{\nu} - \zeta_{\mathbf{k}} - \eta_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\begin{pmatrix} i\omega_{\nu} - \zeta_{\mathbf{k}} - \eta_{\mathbf{k}} & \pm \Delta \\ \pm \Delta & i\omega_{\nu} - \zeta_{\mathbf{k}} + \eta_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} G_{\sigma}(\mathbf{k}, i\omega_{\nu}) \\ \tilde{G}_{\sigma}(\mathbf{k}, i\omega_{\nu}) \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}.$$

The matrix on the l.h.s. can be written as (with 1:  $2 \times 2$  unit matrix,  $\tau$ : Pauli matrices)

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One can show (Landau-Lifshitz, Quantum Mechanics) that for any a and any vector b:

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In our case  $a = i\omega_{\nu} - \zeta_k$ ,  $b = (\pm\Delta, 0, -\eta_k)$  Therefore

$$\begin{pmatrix} G_{\sigma}(\mathbf{k}, i\omega_{\nu}) \\ \tilde{G}_{\sigma}(\mathbf{k}, i\omega_{\nu}) \end{pmatrix} = \frac{1}{(i\omega_{\nu} - \zeta_{\mathbf{k}})^2 - (\Delta^2 + \eta_{\mathbf{k}}^2)} \begin{pmatrix} i\omega_{\nu} - \zeta_{\mathbf{k}} + \eta_{\mathbf{k}} \\ \mp \Delta \end{pmatrix}$$

$$\begin{pmatrix} G_{\sigma}(\mathbf{k}, i\omega_{\nu}) \\ \tilde{G}_{\sigma}(\mathbf{k}, i\omega_{\nu}) \end{pmatrix} = \frac{1}{(i\omega_{\nu} - \zeta_{\mathbf{k}})^2 - (\Delta^2 + \eta_{\mathbf{k}}^2)} \begin{pmatrix} i\omega_{\nu} - \zeta_{\mathbf{k}} + \eta_{\mathbf{k}} \\ \mp \Delta \end{pmatrix}$$

$$\begin{aligned} \boldsymbol{\zeta}_{\boldsymbol{k}} &= \frac{1}{2} \left( \tilde{\boldsymbol{\epsilon}}_{\mathbf{k}} + \tilde{\boldsymbol{\epsilon}}_{\mathbf{k}+\mathbf{Q}} \right), & \eta_{\boldsymbol{k}} &= \frac{1}{2} \left( \tilde{\boldsymbol{\epsilon}}_{\mathbf{k}} - \tilde{\boldsymbol{\epsilon}}_{\mathbf{k}+\mathbf{Q}} \right), \\ \tilde{\boldsymbol{\epsilon}}_{\mathbf{k}} &= \boldsymbol{\epsilon}_{\mathbf{k}} + \frac{n_e U}{2} - \mu & \Delta &= \frac{mU}{2} \end{aligned}$$

Reminder:

- This is the complete solution for given  $n_e$ ,  $\mu$  and m
- The Green's function can be analytically continued  $i\omega_{\nu} \rightarrow \omega$ ,  $\omega$  complex
- Both Green's function have simple poles (=quasiparticle energies) when  $(\omega \zeta_k)^2 (\Delta^2 + \eta_k^2) = 0$

$$\Rightarrow \omega = E_{\mathbf{k}}^{(\pm)} = \zeta_{\mathbf{k}} \pm W_{\mathbf{k}} \qquad \qquad W_{\mathbf{k}} = \sqrt{\Delta^2 + \eta_{\mathbf{k}}^2}$$

- For each **k** there are two poles  $E_{k}^{(\pm)} \Rightarrow$  two 'bands' rather than one
- It is straightforward to show that the bands obey  $E_{k+Q}^{(\pm)} = E_{k}^{(\pm)}$  (with  $Q = (\frac{\pi}{a}, \frac{\pi}{a})$ )

The Green's function was

$$G_{\sigma}(\mathbf{k},\omega) = \frac{\omega - \zeta_{\mathbf{k}} + \eta_{\mathbf{k}}}{(\omega - \zeta_{\mathbf{k}})^2 - (\Delta^2 + \eta_{\mathbf{k}}^2)} = \frac{Z_{\mathbf{k}}^{(-)}}{\omega - E_{\mathbf{k}}^{(-)}} + \frac{Z_{\mathbf{k}}^{(+)}}{\omega - E_{\mathbf{k}}^{(+)}}$$

with

$$E_{\mathbf{k}}^{(\pm)} = \zeta_{\mathbf{k}} \pm W_{\mathbf{k}} \qquad \qquad Z_{\mathbf{k}}^{(\pm)} = \frac{1}{2} \left( 1 \pm \frac{\eta_{\mathbf{k}}}{W_{\mathbf{k}}} \right)$$

We can now obtain the single particle spectral function (=combined photoemission and inverse photoemission spectrum)  $A(\mathbf{k}, \omega)$  by analytical continuation  $i\omega_{\nu} \rightarrow \omega + i\epsilon$  and using

$$\lim_{\epsilon \to 0} \mathcal{I} \frac{1}{\omega + i\epsilon} = -\pi \,\delta(\omega)$$

we get

$$A(\mathbf{k},\omega) = -\frac{1}{\pi} \lim_{\epsilon \to 0} \mathcal{I} G_{\sigma}(\mathbf{k},\omega+i\epsilon) = Z_{\mathbf{k}}^{(-)} \,\delta(\omega - E_{\mathbf{k}}^{(-)}) + Z_{\mathbf{k}}^{(+)} \,\delta(\omega - E_{\mathbf{k}}^{(+)})$$

Combined Photoemission and inverse Photoemission spectrum



In experiment:

## 'Remnant Fermi surface'



$$\begin{pmatrix} G_{\sigma}(\mathbf{k}, i\omega_{\nu}) \\ \tilde{G}_{\sigma}(\mathbf{k}, i\omega_{\nu}) \end{pmatrix} = \frac{1}{(i\omega_{\nu} - \zeta_{\mathbf{k}})^2 - (\Delta^2 + \eta_{\mathbf{k}}^2)} \begin{pmatrix} i\omega_{\nu} - \zeta_{\mathbf{k}} + \eta_{\mathbf{k}} \\ \mp \Delta \end{pmatrix}$$
$$\frac{\zeta_{\mathbf{k}}}{\mp \Delta} = \frac{1}{2} (\tilde{\epsilon}_{\mathbf{k}} + \tilde{\epsilon}_{\mathbf{k}+\mathbf{Q}}), \qquad \eta_{\mathbf{k}} = \frac{1}{2} (\tilde{\epsilon}_{\mathbf{k}} - \tilde{\epsilon}_{\mathbf{k}+\mathbf{Q}}),$$
$$\tilde{\epsilon}_{\mathbf{k}} = \epsilon_{\mathbf{k}} + \frac{n_e U}{2} - \mu \qquad \Delta = \frac{mU}{2}$$

Reminder:

- This is the complete solution for given  $n_e\text{, }\mu$  and m

We recall the definition of the Green's functions...

$$G_{\sigma}(\mathbf{k},\tau) = -\langle T c_{\mathbf{k},\sigma}(\tau) c_{\mathbf{k},\sigma}^{\dagger} \rangle \qquad \qquad \tilde{G}_{\sigma}(\mathbf{k},\tau) = -\langle T c_{\mathbf{k}+\mathbf{Q},\sigma}(\tau) c_{\mathbf{k},\sigma}^{\dagger} \rangle$$

.. and the expectation values (for any site i !)

$$\langle n_{i,\uparrow} \rangle = \frac{n_e}{2} + \frac{m}{2} e^{i \mathbf{Q} \cdot \mathbf{R}_i} \qquad n_e = \langle n_{i,\uparrow} + n_{i,\downarrow} \rangle,$$

$$\langle n_{i,\downarrow} \rangle = \frac{n_e}{2} - \frac{m}{2} e^{i \mathbf{Q} \cdot \mathbf{R}_i}$$
  $m = \langle n_{i,\uparrow} - n_{i,\downarrow} \rangle e^{i \mathbf{Q} \cdot \mathbf{R}_i}$ 

We sum this over i, divide by N, and switch to Fourier transformed c-operators:

$$\begin{split} n_e &= \frac{1}{N} \sum_{\mathbf{k}} \left\langle \ c^{\dagger}_{\mathbf{k},\uparrow} c_{\mathbf{k},\uparrow} + c^{\dagger}_{\mathbf{k},\downarrow} c_{\mathbf{k},\downarrow} \right\rangle \\ m &= \frac{1}{N} \sum_{\mathbf{k}} \left\langle \ c^{\dagger}_{\mathbf{k},\uparrow} c_{\mathbf{k},\uparrow} - c^{\dagger}_{\mathbf{k},\downarrow} c_{\mathbf{k}+\mathbf{Q},\downarrow} \right\rangle = \frac{1}{N} \sum_{\mathbf{k}} \left( \ \tilde{G}_{\uparrow}(\mathbf{k},\tau=0^{-}) + G_{\downarrow}(\mathbf{k},\tau=0^{-}) \right) \\ \end{split}$$

We recall (upper sign for  $\sigma = \uparrow$ )

$$\begin{pmatrix} G_{\sigma}(\mathbf{k}, i\omega_{\nu}) \\ \tilde{G}_{\sigma}(\mathbf{k}, i\omega_{\nu}) \end{pmatrix} = \frac{1}{(i\omega_{\nu} - \zeta_{\mathbf{k}})^2 - (\Delta^2 + \eta_{\mathbf{k}}^2)} \begin{pmatrix} i\omega_{\nu} - \zeta_{\mathbf{k}} + \eta_{\mathbf{k}} \\ \mp \Delta \end{pmatrix}$$
We recall the definition of the Green's functions...

$$G_{\sigma}(\mathbf{k},\tau) = -\langle T c_{\mathbf{k},\sigma}(\tau) c_{\mathbf{k},\sigma}^{\dagger} \rangle \qquad \qquad \tilde{G}_{\sigma}(\mathbf{k},\tau) = -\langle T c_{\mathbf{k}+\mathbf{Q},\sigma}(\tau) c_{\mathbf{k},\sigma}^{\dagger} \rangle$$

.. and the expectation values (for any site i !)

$$\langle n_{i,\uparrow} \rangle = \frac{n_e}{2} + \frac{m}{2} e^{i \mathbf{Q} \cdot \mathbf{R}_i} \qquad n_e = \langle n_{i,\uparrow} + n_{i,\downarrow} \rangle,$$

$$\langle n_{i,\downarrow} \rangle = \frac{n_e}{2} - \frac{m}{2} e^{i \mathbf{Q} \cdot \mathbf{R}_i}$$
  $m = \langle n_{i,\uparrow} - n_{i,\downarrow} \rangle e^{i \mathbf{Q} \cdot \mathbf{R}_i}$ 

We sum this over i, divide by N, and switch to Fourier transformed c-operators:

$$\begin{split} n_e &= \frac{1}{N} \sum_{\mathbf{k}} \left\langle \ c^{\dagger}_{\mathbf{k},\uparrow} c_{\mathbf{k},\uparrow} + c^{\dagger}_{\mathbf{k},\downarrow} c_{\mathbf{k},\downarrow} \right\rangle \\ m &= \frac{1}{N} \sum_{\mathbf{k}} \left\langle \ c^{\dagger}_{\mathbf{k},\uparrow} c_{\mathbf{k},\uparrow} - c^{\dagger}_{\mathbf{k},\downarrow} c_{\mathbf{k}+\mathbf{Q},\downarrow} \right\rangle = \frac{1}{N} \sum_{\mathbf{k}} \left( \ \tilde{G}_{\uparrow}(\mathbf{k},\tau=0^{-}) + G_{\downarrow}(\mathbf{k},\tau=0^{-}) \right) \\ \end{split}$$

We recall the definition of the Green's functions...

$$G_{\sigma}(\mathbf{k},\tau) = -\langle T c_{\mathbf{k},\sigma}(\tau) c_{\mathbf{k},\sigma}^{\dagger} \rangle \qquad \qquad \tilde{G}_{\sigma}(\mathbf{k},\tau) = -\langle T c_{\mathbf{k}+\mathbf{Q},\sigma}(\tau) c_{\mathbf{k},\sigma}^{\dagger} \rangle$$

.. and the expectation values (for any site i !)

$$\langle n_{i,\uparrow} \rangle = \frac{n_e}{2} + \frac{m}{2} e^{i \mathbf{Q} \cdot \mathbf{R}_i} \qquad n_e = \langle n_{i,\uparrow} + n_{i,\downarrow} \rangle,$$

$$\langle n_{i,\downarrow} \rangle = \frac{n_e}{2} - \frac{m}{2} e^{i \mathbf{Q} \cdot \mathbf{R}_i}$$
  $m = \langle n_{i,\uparrow} - n_{i,\downarrow} \rangle e^{i \mathbf{Q} \cdot \mathbf{R}_i}$ 

We sum this over i, divide by N, and switch to Fourier transformed c-operators:

$$n_{e} = \frac{1}{N} \sum_{\mathbf{k}} \left\langle c_{\mathbf{k},\uparrow}^{\dagger} c_{\mathbf{k},\uparrow} + c_{\mathbf{k},\downarrow}^{\dagger} c_{\mathbf{k},\downarrow} \right\rangle = \frac{2}{N} \sum_{\mathbf{k}} G_{\uparrow}(\mathbf{k},\tau=0^{-})$$
$$m = \frac{1}{N} \sum_{\mathbf{k}} \left\langle c_{\mathbf{k},\uparrow}^{\dagger} c_{\mathbf{k}+\mathbf{Q},\uparrow} - c_{\mathbf{k},\downarrow}^{\dagger} c_{\mathbf{k}+\mathbf{Q},\downarrow} \right\rangle = \frac{2}{N} \sum_{\mathbf{k}} \tilde{G}_{\uparrow}(\mathbf{k},\tau=0^{-})$$

The Green's functions at infinitesimally negative  $\tau$  can be evaluated using contour integration techniques After some calculations (see the lecture notes) we obtain the self-consistency equations

$$n_e = \frac{2}{N} \sum_{\mathbf{k}} \left( f(E_{\mathbf{k}}^{(-)}) Z_{\mathbf{k}}^{(-)} + f(E_{\mathbf{k}}^{(+)}) Z_{\mathbf{k}}^{(+)} \right)$$
(2)

$$1 = \frac{U}{N} \sum_{\mathbf{k}} \frac{1}{2W_{\mathbf{k}}} \left( f(E_{\mathbf{k}}^{-}) - f(E_{\mathbf{k}}^{+}) \right)$$
(3)

with  $W_{m k}=\sqrt{\Delta^2+\eta_{m k}^2}$ 

$$E_{\mathbf{k}}^{(\pm)} = \zeta_{\mathbf{k}} \pm W_{\mathbf{k}} \qquad \qquad Z_{\mathbf{k}}^{(\pm)} = \frac{1}{2} \left( 1 \pm \frac{\eta_{\mathbf{k}}}{W_{\mathbf{k}}} \right)$$
$$\zeta_{\mathbf{k}} = \frac{1}{2} \left( \tilde{\epsilon}_{\mathbf{k}} + \tilde{\epsilon}_{\mathbf{k}+\mathbf{Q}} \right), \qquad \qquad \eta_{\mathbf{k}} = \frac{1}{2} \left( \tilde{\epsilon}_{\mathbf{k}} - \tilde{\epsilon}_{\mathbf{k}+\mathbf{Q}} \right),$$
$$\tilde{\epsilon}_{\mathbf{k}} = \epsilon_{\mathbf{k}} + \frac{n_{e}U}{2} - \mu \qquad \qquad \Delta = \frac{mU}{2}$$

 $Z_k$  and  $E_k$  depend on  $\mu$  and  $m \Rightarrow$  for given  $n_e$  and T we solve this by a self-consistency procedure Choose  $m_{in}$  - Determine  $\mu$  from (1) - vary  $m_{in}$  until (2) is satisfied

Results of solving the the self-consistency equations



• Vanishing of m - AF phase transition - for increasing temperature/decreasing electron density

• Fermi surface is an elliptical hole pocket centered on  $(\frac{\pi}{2}, \frac{\pi}{2})$ 

## Summary, Spin density wave theory

- Basic physical idea: assume static antiferromagnetically ordered moments
- Predicts antiferromagnetic insulator at half-filling
- Insulating gap  $\propto$  ordered moment
- Mean-field theory self-energy reduces to the Hartree-Fock potential
- At the antiferromagnetic transition the gap closes the system becomes an ordinary metal
- For the lightly doped case the Fermi surface is an elliptical hole pocket centered on  $(\frac{\pi}{2}, \frac{\pi}{2})$
- Fractional area of hole pockets is  $1 n_e$  MIT by vanishing carrier number

The above derivation closely parallels Gorkov's re-derivation of BCS theory in terms of imaginary-time Green's function

The only Difference is that in the case of BCS theory the anomalous Green's function is  $\tilde{G}(\mathbf{k}, \tau) = -\langle T c_{\mathbf{k},\uparrow}(\tau) c_{-\mathbf{k},\downarrow} \rangle$ The formulation in terms of Green's functions allows to treat spatial inhomogeneity (Landau-Ginzburg theory) systems with impurities (gapless superconductivity) and to go beyond simple BCS theory (Eliashberg theory)