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The Two-Dimensional Hubbard Model

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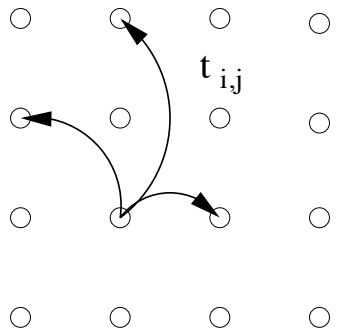
The Hubbard model

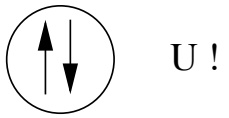
- This model was introduced in the 60's to describe 3d transition metal compounds
- It was very intensively studied following the discovery of cuprate superconductors

$$H = \sum_{i,j} \sum_{\sigma} t_{i,j}\, c^{\dagger}_{i,\sigma} c_{j,\sigma} + U \sum_{i} n_{i,\uparrow}\, n_{i,\downarrow}$$

$$= \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}}\, c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + U \sum_{i} n_{i,\uparrow}\, n_{i,\downarrow}$$

$$\epsilon_{\mathbf{k}} = \frac{1}{N} \sum_{i,j} e^{i\mathbf{k}\cdot(\mathbf{R}_i - \mathbf{R}_j)}$$





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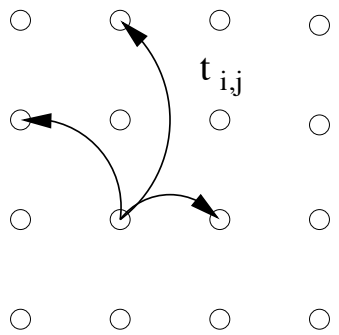
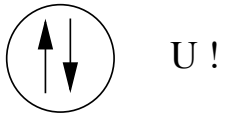




A very important additional parameter in this model is the density of electrons

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 cuprate supercondutors the important range of densities is $1 \geq n_e \geq 0.7$ 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

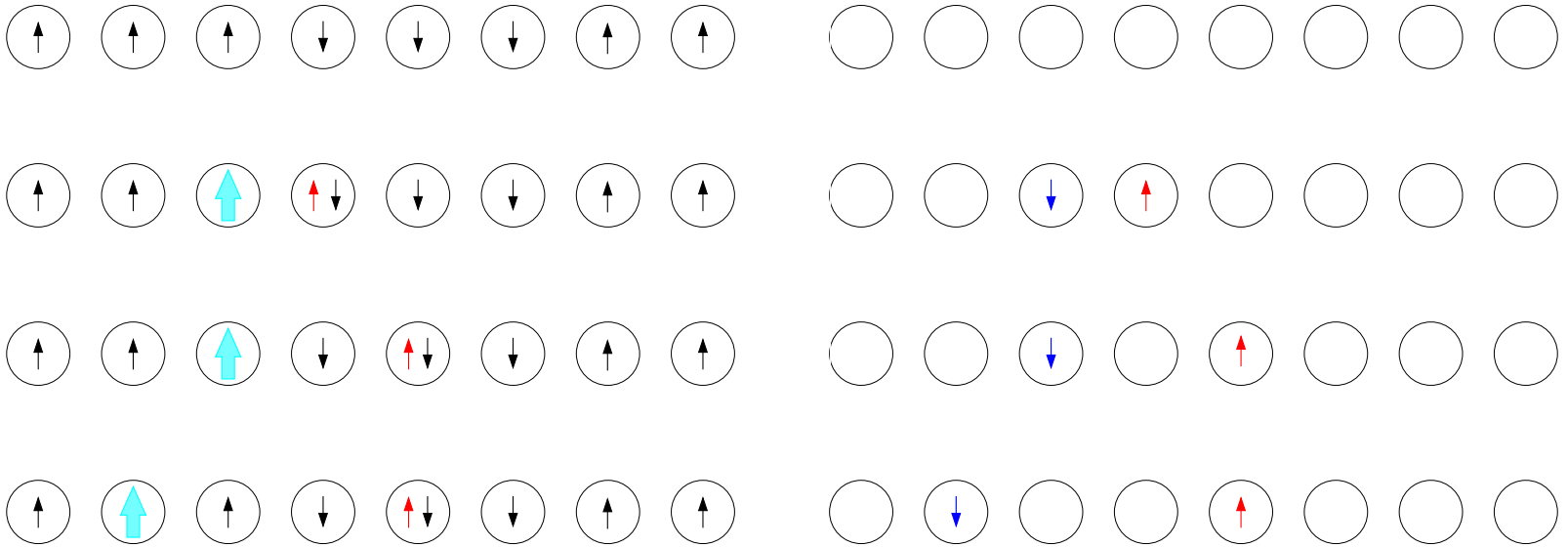
The Hubbard-I approximation

- 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

$$n_{deg} = \begin{pmatrix} N \\ N/2 \end{pmatrix}$$

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

Charge fluctuations as Fermionic Particles



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

Fourier transformation gives

$$H \;=\; \sum_{\mathbf{k},\sigma} \Big((\frac{\epsilon_{\mathbf{k}}}{2} + U)\; d^{\dagger}_{\mathbf{k},\sigma} d_{\mathbf{k},\sigma} - \frac{\epsilon_{\mathbf{k}}}{2}\; h^{\dagger}_{\mathbf{k},\sigma} h_{\mathbf{k},\sigma} \Big) + \sum_{\mathbf{k},\sigma} \frac{\epsilon_{\mathbf{k}}}{2} \Big(d^{\dagger}_{\mathbf{k},\sigma} h^{\dagger}_{-\mathbf{k},-\sigma} + H.c. \Big)$$

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

$$\begin{aligned} \gamma_{-,\mathbf{k},\sigma} &= \;\; u_{\mathbf{k}}\; d_{\mathbf{k},\sigma} + v_{\mathbf{k}}\; h^{\dagger}_{-\mathbf{k},-\sigma} \\ \gamma_{+,\mathbf{k},\sigma} &= -v_{\mathbf{k}}\; d_{\mathbf{k},\sigma} + u_{\mathbf{k}}\; h^{\dagger}_{-\mathbf{k},-\sigma} \end{aligned} \qquad (1)$$

Demanding...

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

... leads to the eigenvalue problem

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

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

So

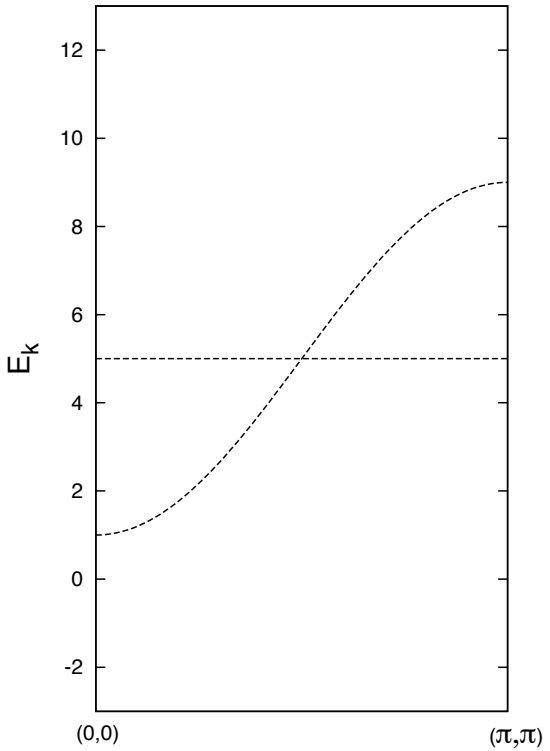
$$E_{\mathbf{k},\pm} = \frac{1}{2}\left(\epsilon_{\mathbf{k}}+U \pm \sqrt{\epsilon_{\mathbf{k}}^2+U^2}\right) \overset{U/t\to\infty}{\longrightarrow} \begin{cases} \frac{\epsilon_{\mathbf{k}}}{2}+U \\ \frac{\epsilon_{\mathbf{k}}}{2} \end{cases}$$

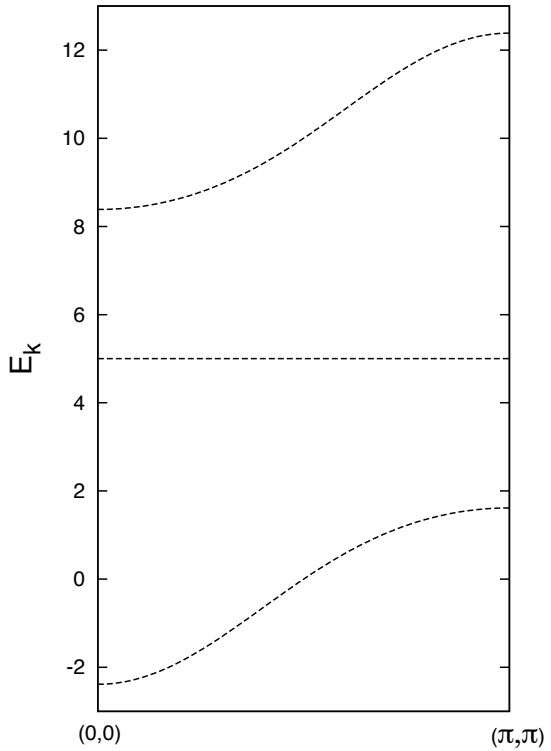
Example: $U/t = 10$

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

Comparison with Hartree-approximation:

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

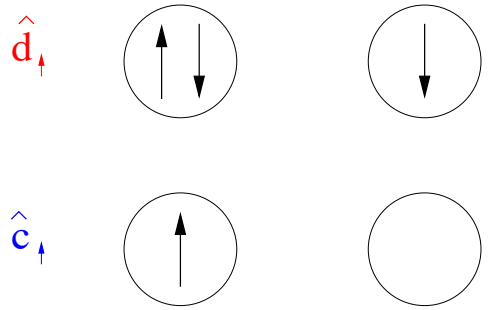




Rigorous Derivation: Equation of motion method

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

$$c_{i,\uparrow} = c_{i,\uparrow}\, n_{i,\downarrow} + c_{i,\uparrow}(1 - n_{i,\downarrow}) = \hat{d}_{i,\uparrow} + \hat{c}_{i,\uparrow}$$



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Accordingly these operators obey

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

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

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

These obey the equations of motion ($\hbar = 1$)

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

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

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

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

$$\begin{aligned}
[\hat{c}_{i,\uparrow}, T_{i,j}] &= [c_{i,\uparrow}\, c_{i,\downarrow}\, c^\dagger_{i,\downarrow}\ ,\ T_{i,j}] \\
&= c_{i,\uparrow}\, c_{i,\downarrow}\, [c^\dagger_{i,\downarrow}, T_{i,j}] + c_{i,\uparrow}\, [c_{i,\downarrow}, T_{i,j}]\, c^\dagger_{i,\downarrow} + [c_{i,\uparrow}, T_{i,j}]\, c_{i,\downarrow}\, c^\dagger_{i,\downarrow} \\
&= t_{i,j}(-c_{i,\uparrow}\, c_{i,\downarrow}\, c^\dagger_{j,\downarrow} + c_{i,\uparrow}\, c_{j,\downarrow}\, c^\dagger_{i,\downarrow} + c_{j,\uparrow}\, c_{i,\downarrow}\, c^\dagger_{i,\downarrow}) \\
&= t_{i,j}(-c_{i,\uparrow}\, c_{i,\downarrow}\, c^\dagger_{j,\downarrow} + c^\dagger_{i,\downarrow}\, c_{i,\uparrow}\, c_{j,\downarrow} + c_{j,\uparrow}\,(\,1 - n_{i,\downarrow}\,)\,) \\
&= t_{i,j}(-c_{i,\uparrow}\, c_{i,\downarrow}\, c^\dagger_{j,\downarrow} + \quad S^-_i \quad\ c_{j,\downarrow} + c_{j,\uparrow}\,(\,1 - \quad\ n_{i,\downarrow} \quad\ )\,) \\
&= t_{i,j}(-c_{i,\uparrow}\, c_{i,\downarrow}\, c^\dagger_{j,\downarrow} + \quad S^-_i \quad\ c_{j,\downarrow} + c_{j,\uparrow}\,(\,1 - (\,\frac{n_i}{2} - S^z_i\,)\,)\,) \\
&= t_{i,j}(-c_{i,\uparrow}\, c_{i,\downarrow}\, c^\dagger_{j,\downarrow} + (\,S^-_i\ c_{j,\downarrow} + S^z_i\ c_{j,\uparrow}\,) + c_{j,\uparrow}\,(\,(\,1 - \frac{\langle n_i \rangle}{2}) - (\,\frac{n_i}{2} - \frac{\langle n_i \rangle}{2}\,)\,)
\end{aligned}$$

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

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

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

The various terms describe

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

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

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

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

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

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

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

Spatial Fourier transformation and adding the commutator with H_U gives

$$
\begin{aligned}
[\,\hat{c}_{\mathbf{k},\uparrow}, H] &= (1-\frac{n_e}{2})\,\epsilon_{\mathbf{k}}\,(\hat{c}_{\mathbf{k},\uparrow}+\hat{d}_{\mathbf{k},\uparrow}) \\
[\hat{d}_{\mathbf{k},\uparrow}, H] &= \frac{n_e}{2}\quad \epsilon_{\mathbf{k}}\,(\hat{c}_{\mathbf{k},\uparrow}+\hat{d}_{\mathbf{k},\uparrow}) \;+\; U\;\hat{d}_{\mathbf{k},\uparrow}
\end{aligned}
$$

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

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

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

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

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

$$
i\partial_t\, G_{\hat{d},\hat{d}}(\vec{k},t) \;=\; \delta(t)\,\langle n_{-\sigma}\rangle + \frac{n_e}{2}\,\epsilon_{\mathbf{k}}\left(\, G_{\hat{c},\hat{d}}(\vec{k},t) + \; G_{\hat{d},\hat{d}}(\vec{k},t)\,\right) + U\; G_{\hat{d},\hat{d}}(\vec{k},t)
$$

After Fourier transformation with respect to time $(i\partial_t \rightarrow \omega)$ 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 2×2 matrix $\mathbf{G}(\mathbf{k},\omega)$

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

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

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 $\mathbf{k}$-independent self-energy $\Sigma(\omega)$ is given by

$$\begin{aligned}\Sigma(\omega) \;&=\; \frac{n_e}{2}\,U + \frac{n_e}{2}\left(1-\frac{n_e}{2}\right)\frac{U^2}{\omega - \left(1-\frac{n_e}{2}\right)U} \\ &=\; \frac{n_e}{2}\,U + \frac{\sigma}{\omega-\zeta}\end{aligned}$$

This is the sum of the Hartree-Fock potential and a term with a single pole

Relation to the heuristic derivation: set $n_e = 1$

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

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Relation to the heuristic derivation: set $n_e = 1$

$$\begin{pmatrix} i\partial_t - \frac{1}{2}\,\epsilon_{\mathbf{k}} & , & -\frac{1}{2}\,\epsilon_{\mathbf{k}} \\ -\frac{1}{2}\,\epsilon_{\mathbf{k}} & , & i\partial_t - \frac{1}{2}\,\epsilon_{\mathbf{k}} - U \end{pmatrix} \begin{pmatrix} G_{\hat{c},\hat{c}} & G_{\hat{c},\hat{d}} \\ G_{\hat{d},\hat{c}} & G_{\hat{d},\hat{d}} \end{pmatrix} \;=\; \delta(t) \begin{pmatrix} \frac{1}{2} & , & 0 \\ 0 & , & \frac{1}{2} \end{pmatrix}$$

Now introduce

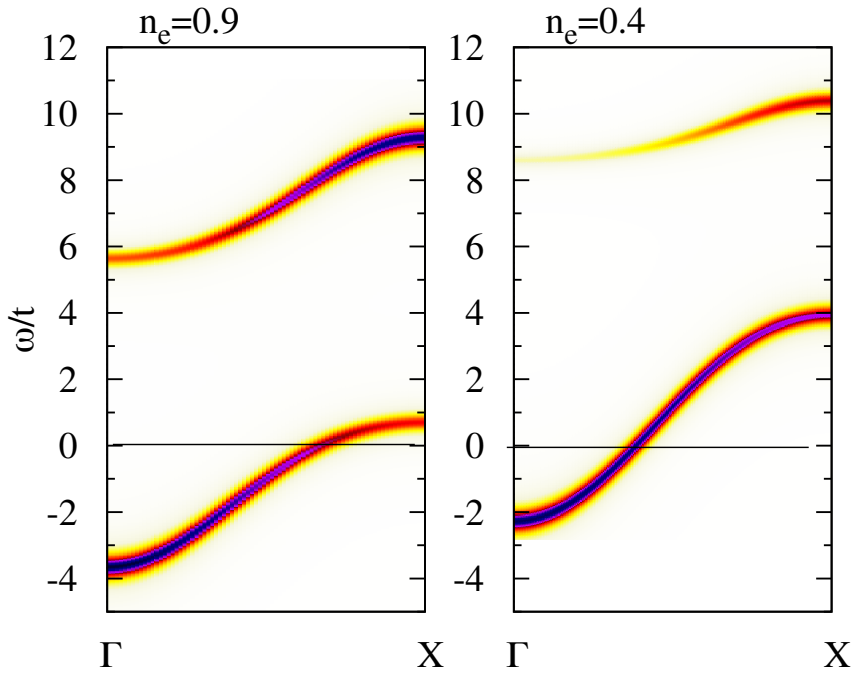
$$\begin{aligned} d^{\dagger}_{i,\sigma} &= \sqrt{2}\;\hat{d}^{\dagger}_{i,\sigma} \\ h^{\dagger}_{i,-\sigma} &= \sqrt{2}\;\hat{c}_{i,\sigma} \end{aligned}$$

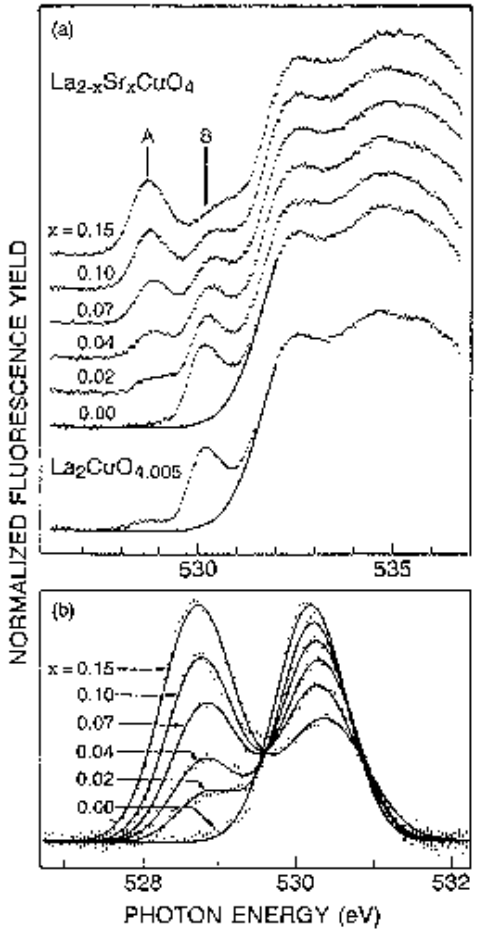
$$\left[i\partial_t - \begin{pmatrix} \frac{1}{2}\,\epsilon_{\mathbf{k}} & , & \frac{1}{2}\,\epsilon_{\mathbf{k}} \\ \frac{1}{2}\,\epsilon_{\mathbf{k}} & , & \frac{1}{2}\epsilon_{\mathbf{k}} + U \end{pmatrix} \right] \begin{pmatrix} -i\langle T\; h^{\dagger}_{-\mathbf{k},\downarrow}(t)\; h_{-\mathbf{k},\downarrow}\rangle & -i\langle T\; h^{\dagger}_{-\mathbf{k},\downarrow}(t)\; d^{\dagger}_{\mathbf{k},\uparrow}\rangle \\ -i\langle T\;\; d_{\mathbf{k},\uparrow}(t)\; h_{-\mathbf{k},\downarrow}\rangle & -i\langle T\;\; d_{\mathbf{k},\uparrow}(t)\; d^{\dagger}_{\mathbf{k},\uparrow}\rangle \end{pmatrix} \;=\; \delta(t)$$

These would also be obtained from the Hamiltonian for the charge fluctuations

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

After fixing the Fermi energy in the usual way we obtain the spectral function

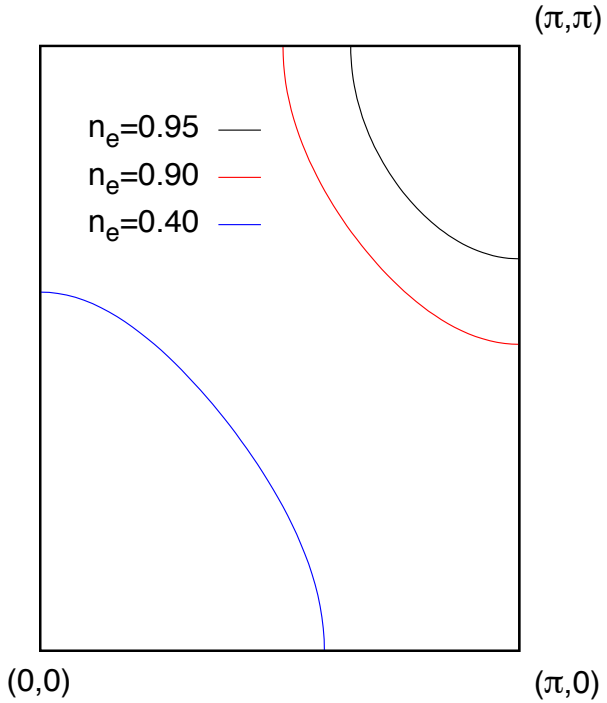


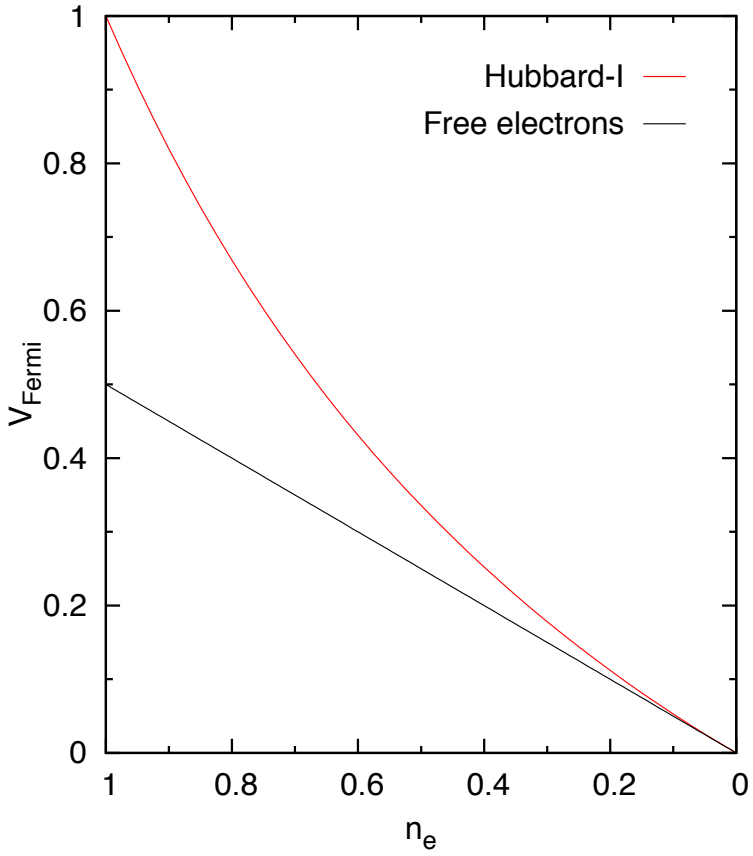


Note the transfer of spectral weight upon decreasing electron density

(Experimental data on $La_{2-x}Sr_xCuO_4$ by C.T. Chen *et al.*, Phys. Rev. Lett. 66, **104** (1991))

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

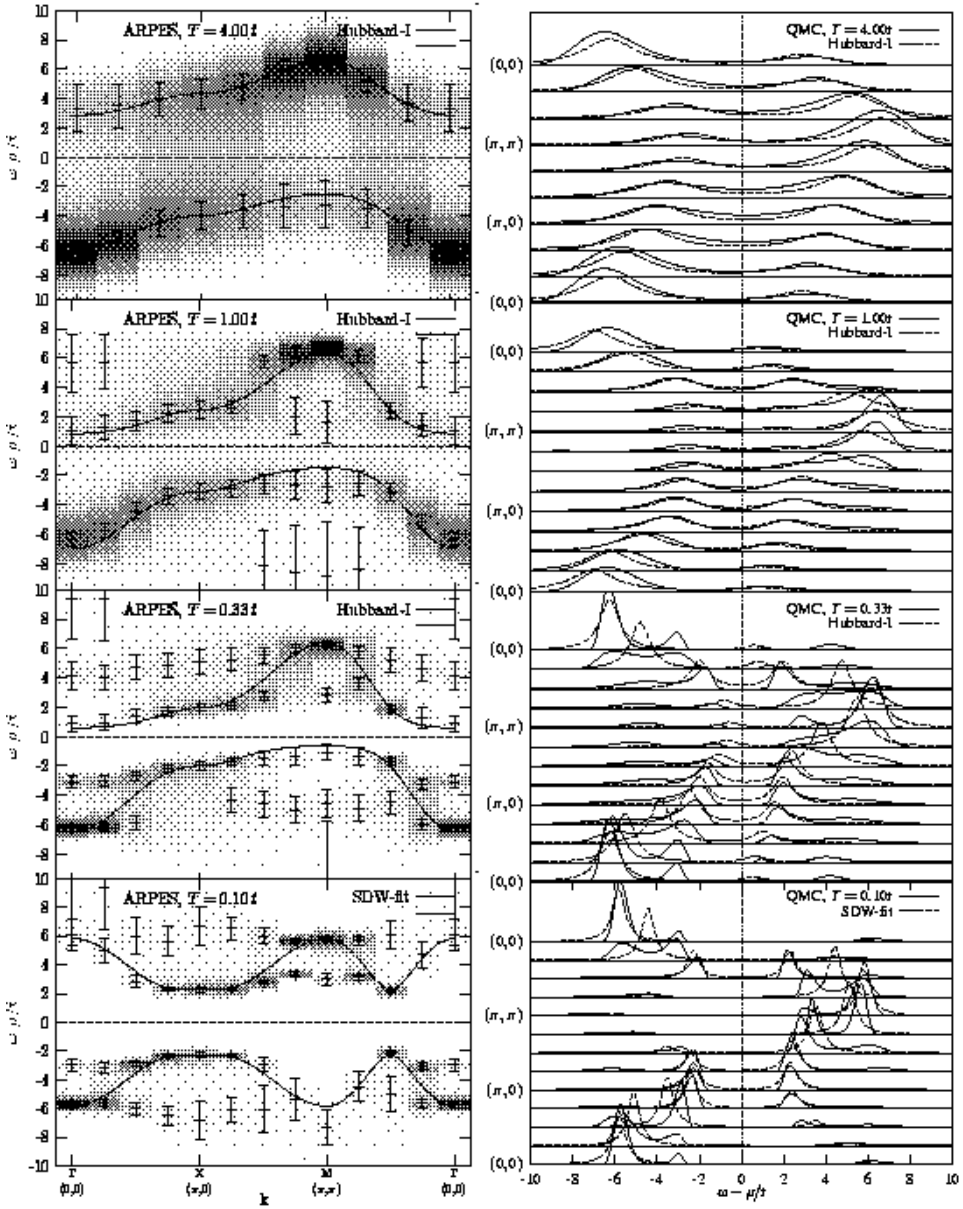




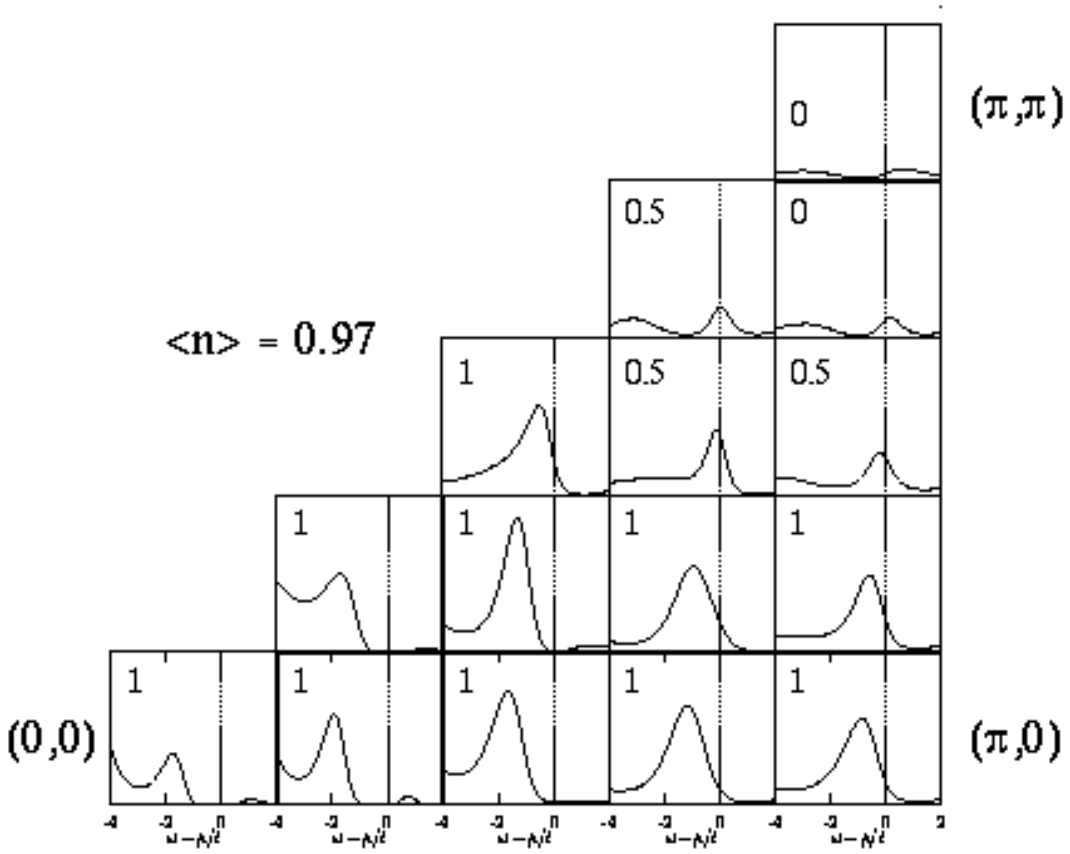
Comparison to $A(\mathbf{k}, \omega)$ obtained by

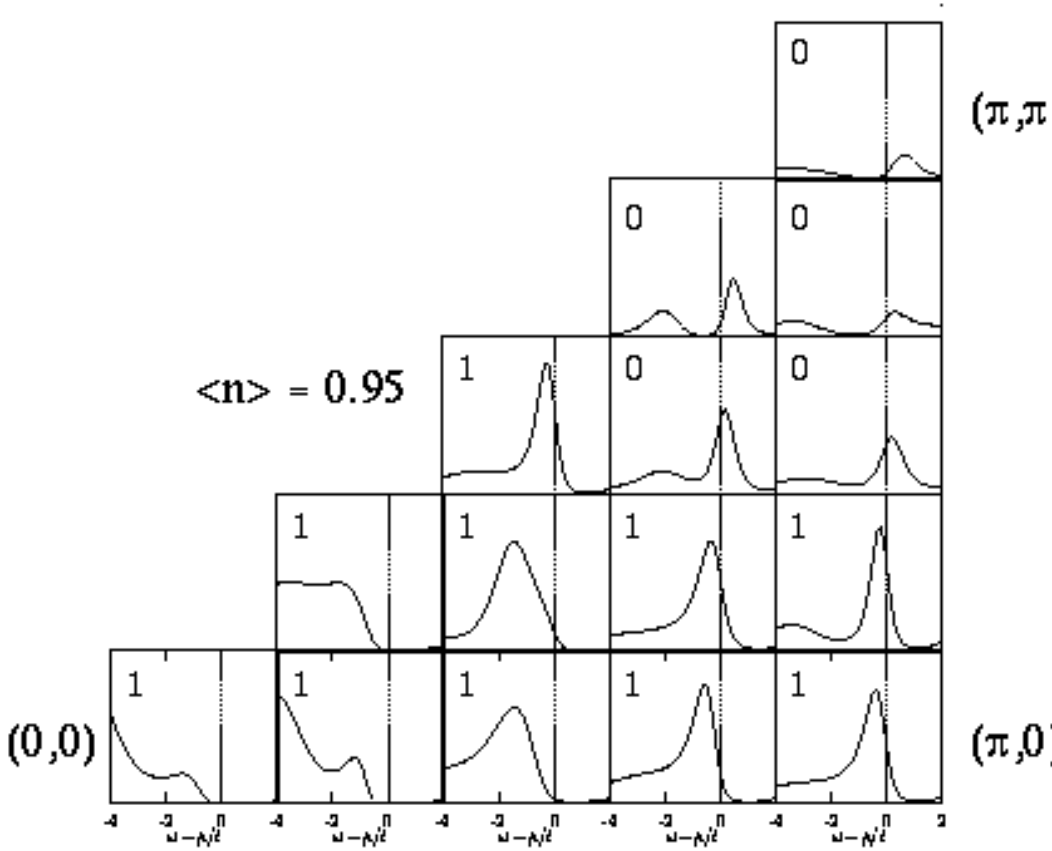
QMC on an 8×8 cluster, $U/t = 8$, $n_e = \frac{1}{2}$

C. Gröber *et al*, PRB $\mathbf{62}$, 4336 (2000).



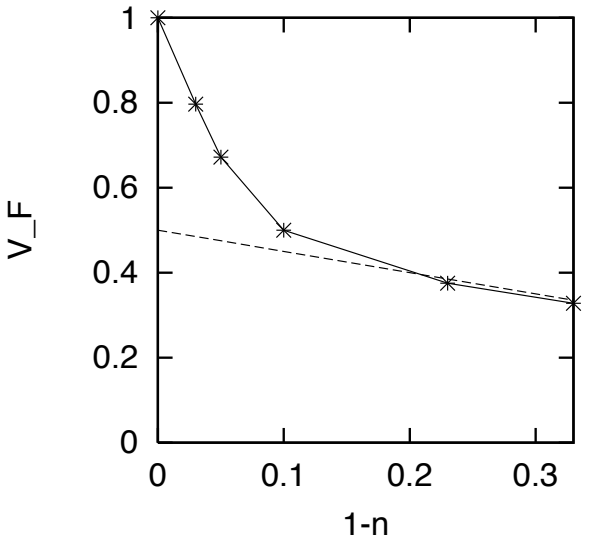
QMC at $k_B T = t$ - Fermi surface volume

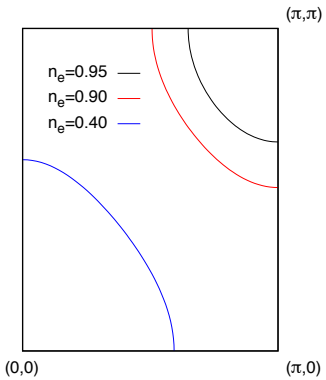


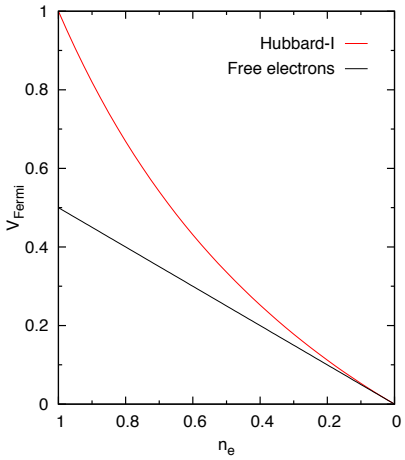


Rough estimate for fractional Fermi surface volume

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







Summary: the Hubbard-I approximation

- Basic step: introduce half-filled state as 'vacuum'
- Charge fluctuations are interpreted as hole-like and double occupany-like 'particles'
- The particles have energies 0 and $U \Rightarrow$ two Hubbard-bands
- For less than half-filling the lower Hubbard band is 'hole doped'
- Fermi surface is a small hole pocket at the maximum of the lower Hubbard band (usually (π, π))
- Fermi surface volume $\rightarrow 0$ as $n_e \rightarrow 1$
- 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

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

- $|FS\rangle$ is the free electron ground state i.e. the Fermi sea
- λ 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

$$\begin{aligned}
(1 - \lambda\; n_\uparrow n_\downarrow) \quad |0\rangle &= |0\rangle \\
(1 - \lambda\; n_\uparrow n_\downarrow) \quad |\uparrow\rangle &= |\uparrow\rangle \\
(1 - \lambda\; n_\uparrow n_\downarrow) \quad |\downarrow\rangle &= |\downarrow\rangle \\
(1 - \lambda\; n_\uparrow n_\downarrow) \quad |\uparrow\downarrow\rangle &= (1-\lambda)|\uparrow\downarrow\rangle
\end{aligned}$$

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!)

$$c^\dagger_{\mathbf{k}} \;=\; \frac{1}{\sqrt{N}} \sum_{j=1}^{N} e^{i\mathbf{k}\cdot\mathbf{R}_j}\, c^\dagger_j$$

Then

$$\prod_{j=1}^{M} c^\dagger_{\mathbf{k}_j}\,|0\rangle \;=\; \frac{1}{\sqrt{N}^M} \sum_{i_1,i_2,i_3,\ldots i_M} exp\left(i \sum_{j=1}^{M} \mathbf{k}_j \cdot \mathbf{R}_{i_j} \right) c^\dagger_{i_1} c^\dagger_{i_2} \ldots c^\dagger_{i_M}|0\rangle$$

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

$$\prod_{j=1}^{M} c^\dagger_{\mathbf{k}_j}\,|0\rangle \;=\; \frac{1}{\sqrt{N}^M} \sum_{i_1>i_2>i_3\cdots>i_M} \sum_{\sigma} exp\left(i \sum_{j=1}^{M} \mathbf{k}_j \cdot \mathbf{R}_{i_{\sigma(j)}} \right) c^\dagger_{i_{\sigma(1)}} c^\dagger_{i_{\sigma(2)}} \ldots c^\dagger_{i_{\sigma(M)}}|0\rangle$$

We had

$$\prod_{j=1}^{M} c^{\dagger}_{\mathbf{k}_j} |0\rangle = \frac{1}{\sqrt{N}^M} \sum_{i_1>i_2>i_3\cdots>i_M} \sum_{\sigma} exp\left(i \sum_{j=1}^{M} \mathbf{k}_j \cdot \mathbf{R}_{i_{\sigma(j)}} \right) c^{\dagger}_{i_{\sigma(1)}} c^{\dagger}_{i_{\sigma(2)}} \dots c^{\dagger}_{i_{\sigma(M)}} |0\rangle$$

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

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

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

$$\begin{aligned} \prod_{j=1}^{M} c^{\dagger}_{\mathbf{k}_j} |0\rangle &= \frac{1}{\sqrt{N}^M} \sum_{i_1>i_2>i_3\cdots>i_M} \sum_{\sigma} (-1)^{\sigma} exp\left(i \sum_{j=1}^{M} \mathbf{k}_j \cdot \mathbf{R}_{i_{\sigma(j)}} \right) c^{\dagger}_{i_1} c^{\dagger}_{i_2} c^{\dagger}_{i_M} |0\rangle \\ &= \frac{1}{\sqrt{N}^M} \sum_{i_1>i_2>i_3\cdots>i_M} D(\mathbf{k}_1, \mathbf{k}_2, \dots, \mathbf{k}_M | i_1, i_2, \dots i_M) \quad c^{\dagger}_{i_1} c^{\dagger}_{i_2} c^{\dagger}_{i_M} |0\rangle \end{aligned}$$

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

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

Since the overlap of any two states with different N_d is zero we have $\langle\Phi(M_d)|\Phi(N_d)\rangle = 0$ for $M_d \neq N_d$

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

Question: which N_d has the largest weight $W(N_d) = \langle\Phi(N_d)|\Phi(N_d)\rangle$ in this sum?

Put another way: Which number of double occupancies is the most probable one?

Remember: $|\Phi(N_d)\rangle$ is the sum over all ordered $N_\uparrow$-tuples $i_1, i_2, \ldots i_{N_\uparrow}$ 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: $(1-\lambda)^{N_d}\, \frac{1}{\sqrt{N}^{N_\uparrow + N_\downarrow}}$

Since any two configurations are orthogonal we only need $D^*(\mathbf{k_j}|i_j)\; D(\mathbf{k_j}|i_j)$

$$\begin{aligned}
D(\mathbf{k}_1, \mathbf{k}_2, \ldots, \mathbf{k}_M | i_1, i_2, \ldots i_M) &= \sum_\sigma (-1)^\sigma \; exp\left(i \sum_{j=1}^{M} \mathbf{k}_j \cdot \mathbf{R}_{i_{\sigma(j)}} \right) \\
D^*(\mathbf{k_j}|i_j)\; D(\mathbf{k_j}|i_j) &= \sum_{\sigma,\sigma'} (-1)^\sigma \; (-1)^{\sigma'} \; exp\left(i \sum_{j=1}^{M} \mathbf{k}_j \cdot (\mathbf{R}_{i_{\sigma(j)}} - \mathbf{R}_{i_{\sigma'(j)}}) \right) \\
&= \sum_\sigma \; 1 + \sum_{\sigma \neq \sigma'} (-1)^\sigma \; (-1)^{\sigma'} \; exp\left(i \sum_{j=1}^{M} \mathbf{k}_j \cdot (\mathbf{R}_{i_{\sigma(j)}} - \mathbf{R}_{i_{\sigma'(j)}}) \right) \\
&= M!
\end{aligned}$$

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?

Now we just found

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

Now: form $\log(W(N_d))$, use Stirling formula...

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

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

...and differentiate with respect to N_d:

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

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

We had

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

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

Now switch to densities $n_\alpha = N_\alpha/N$, $\alpha \in \uparrow, \downarrow, d$

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

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

The first equation gives us the value of $n_d = N_d/N$ where $\langle\Phi(N_d)|\Phi(N_d)\rangle$ is a maximum:

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

The first equation gives us the value of $n_d = N_d/N$ where $\langle \Phi(N_d) | \Phi(N_d) \rangle$ is a maximum:

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

For general n_σ 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!

The second equation was

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

Here c is of order unity

Taylor expansion of the logarithm gives (remember: $n_d = N_d/N \rightarrow N_d = N \cdot n_d$)

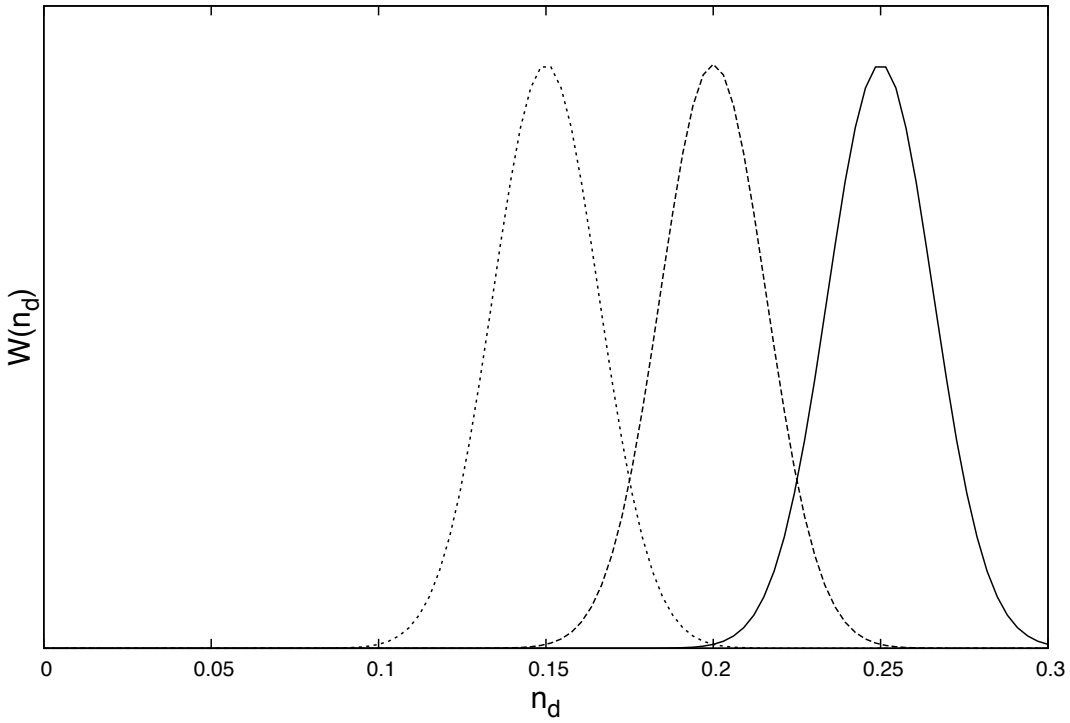
$$\log\left(W(N_d)\right) \;=\; \log\left(W(N_{d,max})\right) - \frac{1}{2}\,\frac{c}{N}\,(N_d - N_{d,max})^2 + \ldots$$

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

$\rightarrow W(n_d)$ is a Gaussian with a width $\propto N^{-1/2}$ as $N \rightarrow \infty$ the width becomes zero

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

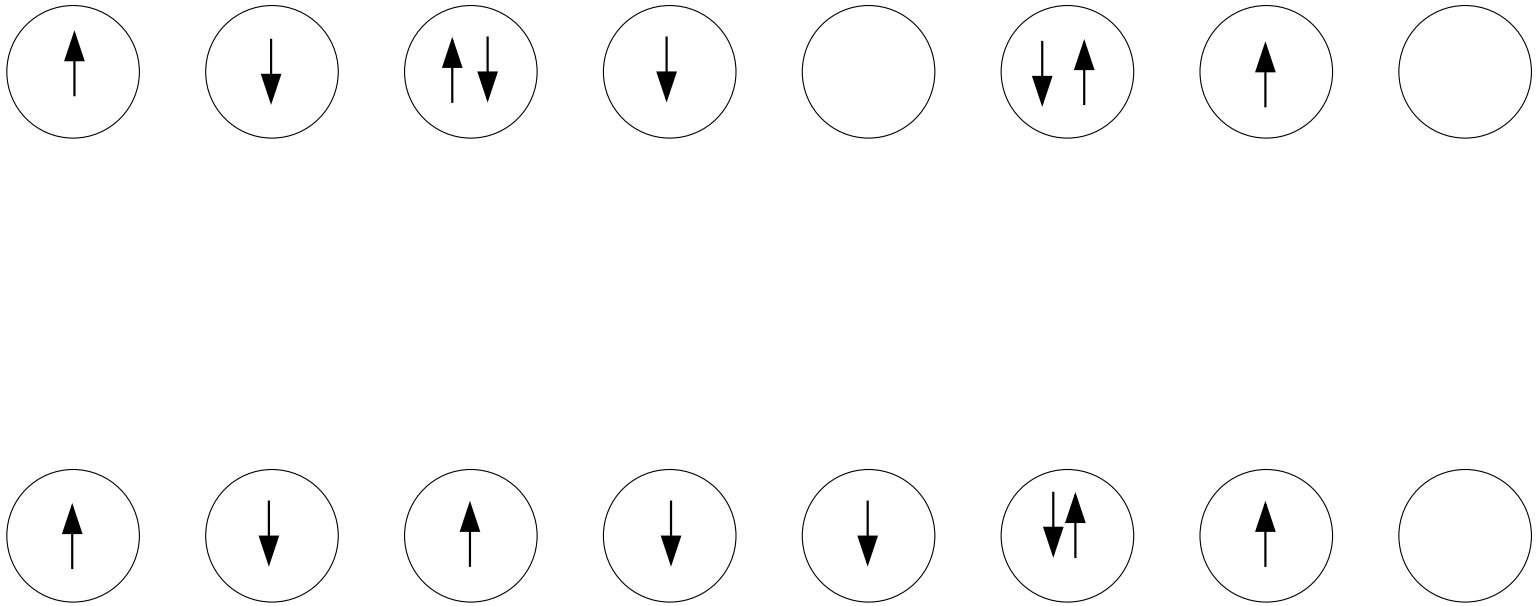
We saw: The whole Gutzwiller wave function consists exclusively of configurations with a fixed $N_d = N \cdot n_d$ and n_d is shifted by varying λ



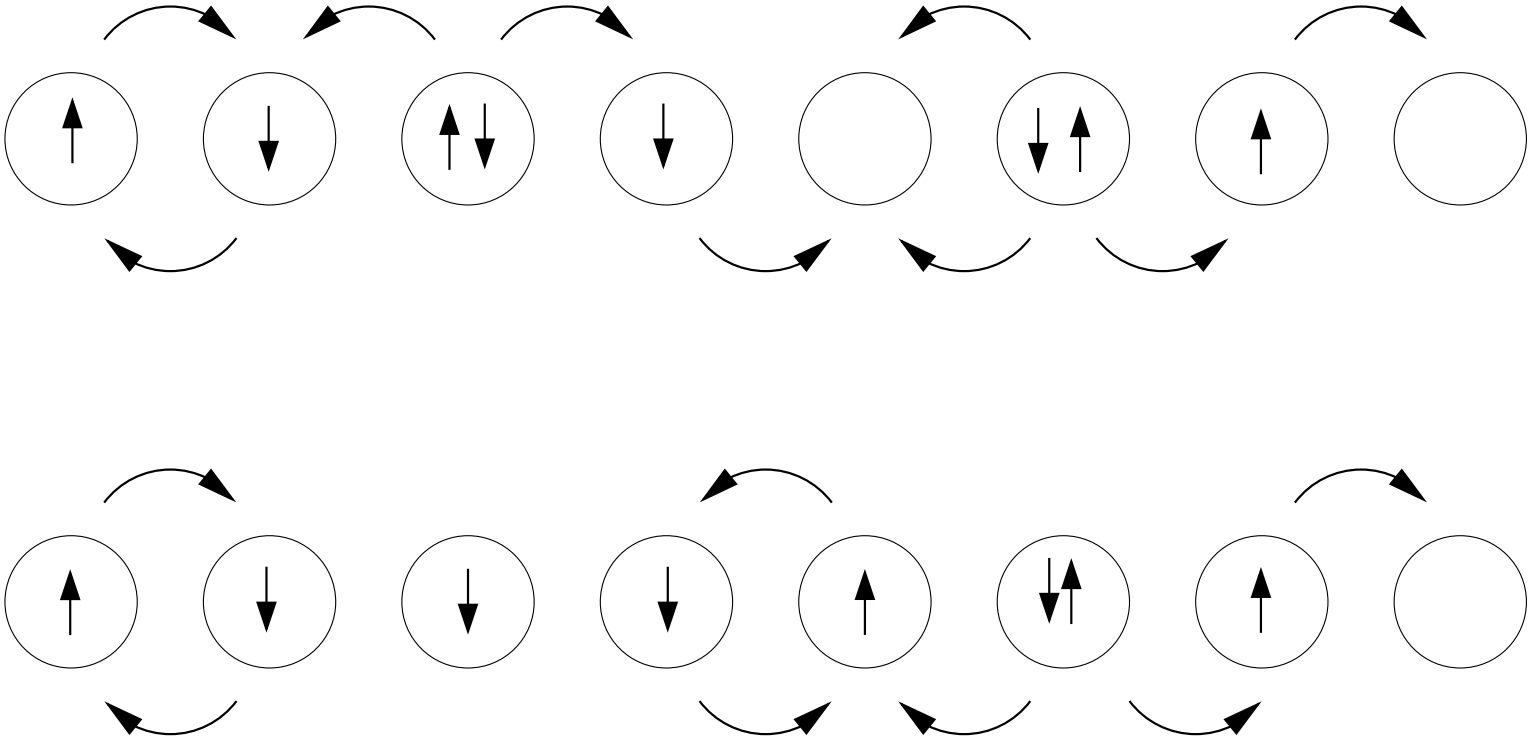
This means, however, that the expectation value of H_U is completely trivial: $\langle H_U \rangle = U \cdot N \cdot n_d$

The expectation value of H_t is more difficult....

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



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 η_σ 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 σ-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 4 'book-keeping kets' for every site i: $|i,0\rangle$, $|i,\uparrow\rangle$, $|i,\downarrow\rangle$ and $|i,\uparrow\downarrow\rangle$

Define the wave function of a single site i (with α_σ, β real).....

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

... and the wave function of the whole lattice

$$
\begin{aligned}
|\Psi\rangle &= \prod_i |B_i\rangle \\
\langle\Psi|\Psi\rangle &= 1
\end{aligned}
$$

We had

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

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

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

which can be reverted to give

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

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

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

$|\Psi\rangle$ has norm 1 and as many 'empty sites', 'singly occupied sites' and 'doubly occupied sites' as the true Gutzwiller wave function if we adjust α_σ and β correctly

But: $|\Psi\rangle$ does not have 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[2]: It is straightforward to show that the values of N_α - with $\alpha \in \{\uparrow, \downarrow, d\}$ have a Gaussian distribution around their mean values $\bar{N}_\alpha$ with a width which is again $\propto N^{-1/2}$

More precisely: if we decompose $|\Psi\rangle$ into components $|\Psi(N_\alpha)\rangle$ of fixed N_α the weight of $|\Psi(N_\alpha)\rangle$ can be shown to be

$$W(N_\alpha) \;=\; A \cdot \exp\left(-c\,\frac{(N_\alpha - \bar{N}_\alpha)^2}{N}\right)$$

Therefore, in calculating expectation values we may replace $|\Psi'\rangle \to |\Psi\rangle$

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

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

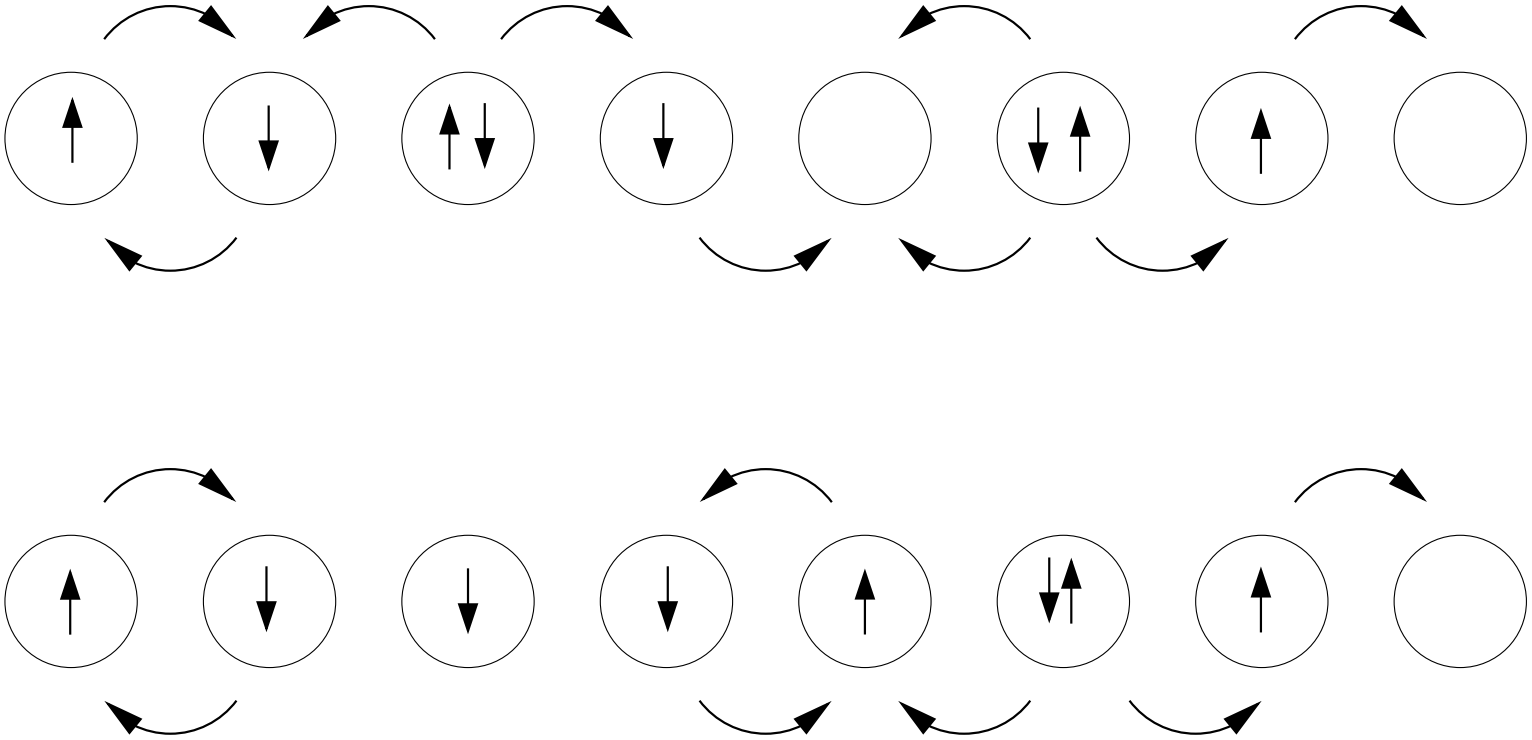
Now we 'translate' the electron operators (note: this ignores the Fermi sign)

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

Then we estimate the number of hopping possibilities per bond as

$$
\begin{aligned}
h(\uparrow, n_\uparrow, n_\downarrow, n_d) &= \frac{\langle\Psi|\tilde{c}_{i,\uparrow}^\dagger \, \tilde{c}_{j,\uparrow}|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \langle\Psi|\tilde{c}_{i,\uparrow}^\dagger \, \tilde{c}_{j,\uparrow}|\Psi\rangle = \langle B_i|\tilde{c}_{i,\uparrow}^\dagger|B_i\rangle \, \langle B_j|\tilde{c}_{j,\uparrow}|B_j\rangle \\
&= |\langle B_i|\tilde{c}_{i,\uparrow}|B_i\rangle|^2 = \left(\frac{\alpha_\uparrow + \alpha_\downarrow\beta}{1+\alpha_\uparrow^2+\alpha_\downarrow^2+\beta^2}\right)^2
\end{aligned}
$$

We remember:



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|\Psi\rangle &= \prod_i |B_i\rangle
\end{aligned}
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&= |\langle B_j|\tilde{c}_{j,\uparrow}|B_j\rangle|^2 = \left(\frac{\alpha_\uparrow + \alpha_\downarrow\beta}{1+\alpha_\uparrow^2+\alpha_\downarrow^2+\beta^2}\right)^2
\end{aligned}
$$

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

But we found earlier that α_σ and β can be expressed by n_σ and n_d....

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

.... 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

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

Collecting everything

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

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

and found the terms of the sum '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 $\lambda \to n_d$ 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

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

where the renormalization factors η_σ are again 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

We had

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

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

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

where t_0 is the noninteracting kinetic energy 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 $n_\sigma = \frac{1}{2}$

$$\begin{aligned} \eta(n_d) \; &= \; 16 \, n_d \, (\frac{1}{2} - n_d) \\ e(n_d) \; &= \; 16 \, n_d \, (\frac{1}{2} - n_d) \, t_0 + U \, n_d \end{aligned}$$

Then we find the optimal n_d

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

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 $t_0 = -1.621\ t \rightarrow U_c = 12.969\ t$

Quasiparticle Dispersion

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. λ') 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 $|\Phi_G(\mathbf{k})\rangle$ amounts to

$$\begin{aligned} e &\to e - \frac{1}{N}\,\tilde{\epsilon_{\mathbf{k}}} \\ t_0 &\to t_0 - \frac{1}{N}\,\epsilon_{\mathbf{k}} \\ n_\uparrow &\to n_\uparrow - \frac{1}{N} \\ n_d &\to n_d + \frac{1}{N}\,\delta n_d \end{aligned}$$

Inserting and expanding gives

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

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

The condition on n_d (i.e. λ') 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 $|\Phi_G(\mathbf{k})\rangle$ amounts to

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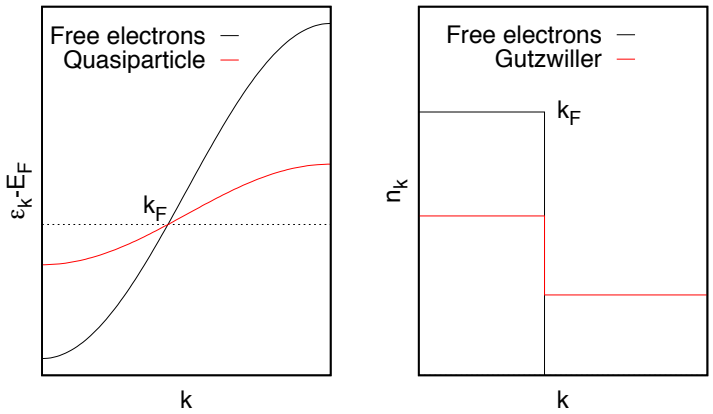
Inserting and expanding gives

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

We thus find that the quasiparticle dispersion is renormalized by the same factor η as the expectation value of the kinetic energy (the constant can be compensated by a shift of μ)

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

Moreover:



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

The Gutzwiller wave function describes the metal insulator transition by the vanishing of the bandwidth

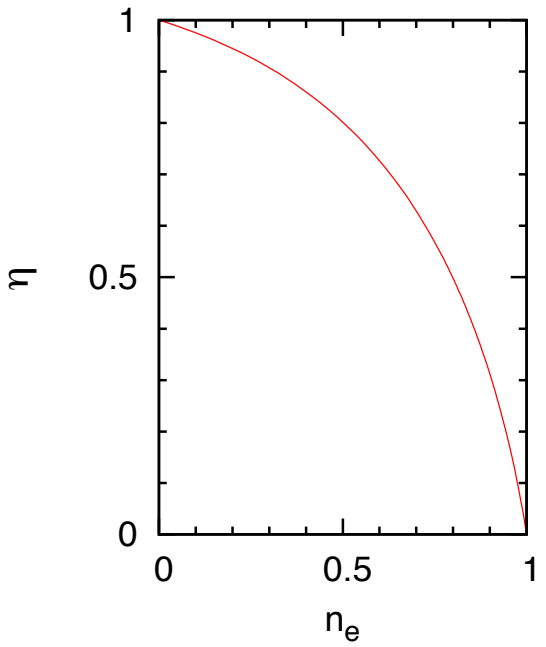
Suppose we have a ratio U/t such that the system is a Mott-insulator at half-filling

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

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, $U/t = 16 > U_c/t = 12.969$)

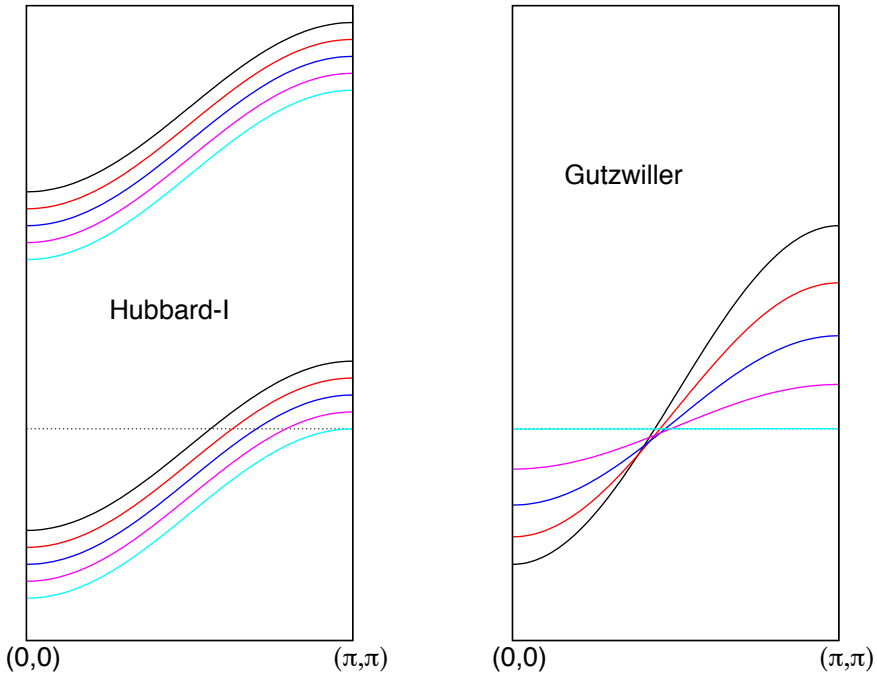


Intermediate Summary: Hubbard-I versus Gutzwiller

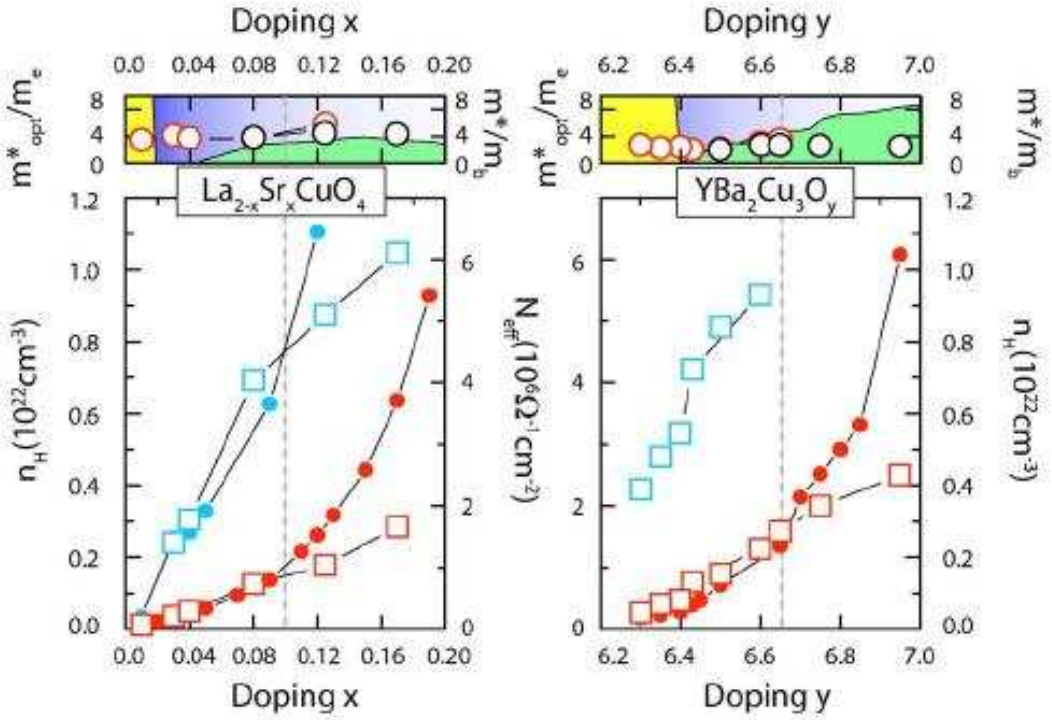
We consider the case of large U/t where the system is a Mott-insulator at half-filling

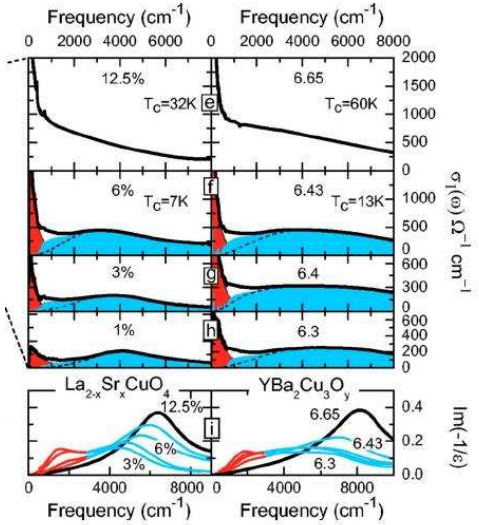
Then we ask: how does the system behave as $n_e \to 1$ from below?

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



Experimentally it seems that Hubbard-I is closer to reality....





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

The Hubbard-I and Gutzwiller approximation are highly oversimplified

We have seen in the derivation of the Hubbard-I approximation that the coupling to spin- and density-excitations - or more generally: the collective excitations of the system - is ignored

This is in fact probably the key problem to be solved.....

For the remainder of the lecture we will discuss this coupling to collective excitations for a special case where a reasonably accurate solution is possible

We will proceed in three steps:

Derive an effective Hamiltonian for the lower Hubbard band

Discuss the collective excitations for the antiferromegnetic phase: magnons

Discuss the effect of the coupling of the magnons to a single mobile hole

It will be seen that the modifications as compared to Hubbard-I are drastic.....

Strong coupling expansion

We consider the Hubbard model in the limit of large U/t

Low energy states will have few double occupancies - another way to say this is that double occupancies exist only as short-lived 'virtual states'

Our goal is to derive an 'effective Hamiltonian' which operates in the subspace of the Hilbert space without double occupancies but takes into account the effect of the short-lived 'virtual states' by suitable correction terms

To that end we use a canonical transformation plus perturbation theory

The Hilbert space can be decomposed into 'sectors' with fixed number of double occupancies

The Hamiltonian can be decomposed into terms which operate within the sectors and terms which connect the sectors

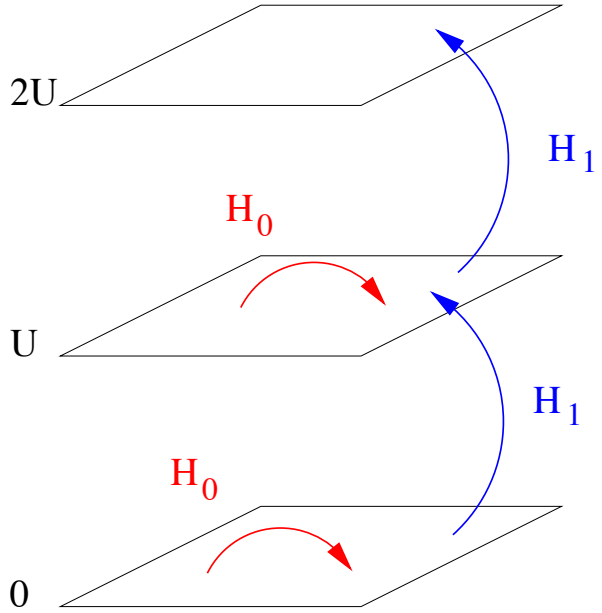
We recall the decomposition of the electron operator familiar from Hubbard-I

$$c_{i,\sigma} \;=\; c_{i,\sigma}\, n_{i,-\sigma} + c_{i,\sigma}(1 - n_{i,-\sigma}) = \hat{d}_{i,\sigma} + \hat{c}_{i,\sigma}$$

$$H \;=\; H_0 + H_1$$

$$H_0 \;=\; \sum_{i,j} \sum_{\sigma} t_{i,j}\, (\hat{c}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} + \hat{d}^{\dagger}_{i,\sigma} \hat{d}_{j,\sigma}) + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow}$$

$$H_1 \;=\; \sum_{i,j} \sum_{\sigma} t_{i,j}\, (\hat{d}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} + \hat{c}^{\dagger}_{i,\sigma} \hat{d}_{j,\sigma})$$



We consider canonical transformations of the Hilbert space

$$|\Psi'\rangle \;=\; e^S\,|\Psi\rangle$$

$$\hat{O}' \;=\; e^S\,\hat{O}\,e^{-S} = \hat{O} + [S,\hat{O}] + \frac{1}{2!}\,[S,[S,\hat{O}]] + \frac{1}{3!}\,[S,[S,[S,\hat{O}]]] + \ldots,$$

Unitarity of e^S requires $S^\dagger = -S$

Example: for $S = \frac{i}{\hbar}\,H\,t$ this is the transformation Schrödinger picture $\rightarrow$ Heisenberg picture

The transformation was

$$|\Psi'\rangle \;=\; e^{S}\,|\Psi\rangle$$

$$\hat{O}' \;=\; e^{S}\,\hat{O}\,e^{-S} = \hat{O} + [S,\hat{O}] + \frac{1}{2!}\,[S,[S,\hat{O}]] + \frac{1}{3!}\,[S,[S,[S,\hat{O}]]] + \ldots,$$

Our goal: Find an S such that 'connecting part' H_1 is eliminated from H'

Insert $\hat{O} \to H_0 + H_1$:

$$H' = H_0 + H_1 + [S,H_0] + [S,H_1] + \frac{1}{2!}\,[S,[S,H_0]] + \frac{1}{2!}\,[S,[S,H_1]] + \ldots$$

The transformation was

$$|\Psi'\rangle \;=\; e^{S}\,|\Psi\rangle$$

$$\hat{O}' \;=\; e^{S}\,\hat{O}\,e^{-S} = \hat{O} + [S,\hat{O}] + \frac{1}{2!}\,[S,[S,\hat{O}]] + \frac{1}{3!}\,[S,[S,[S,\hat{O}]]] + \ldots,$$

Our goal: Find some S such that 'connecting part' H_1 is eliminated from H'

Insert $\hat{O} \to H_0 + H_1$:

$$H' = H_0 + H_1 + [S,H_0] + [S,H_1] + \frac{1}{2!}\,[S,[S,H_0]] + \frac{1}{2!}\,[S,[S,H_1]] + \ldots$$

Now choose S such that

$$H_1 + [S,H_0] = 0$$

Then H' becomes (using $[S, H_0] = -H_1$)

$$H' = H_0 + [S, H_1] + \frac{1}{2!}[S, [S, H_0]] + \frac{1}{2!}[S, [S, H_1]] + \frac{1}{3!}[S, [S, [S, H_0]]] + \ldots$$

$$= H_0 + \frac{1}{2}[S, H_1] + \frac{1}{3}[S, [S, H_1]] + \ldots$$

Obviously this makes sense only if S is 'small' in some sense so that higher order terms can be neglected

In our application to the Hubbard model we had (remember: $U \gg t_{i,j}$)

$$H_0 = \sum_{i,j}\sum_{\sigma} t_{i,j}\ (\hat{c}^{\dagger}_{i,\sigma}\hat{c}_{j,\sigma} + \hat{d}^{\dagger}_{i,\sigma}\hat{d}_{j,\sigma}) + U\sum_{i} n_{i,\uparrow}n_{i,\downarrow} \approx U\sum_{i} n_{i,\uparrow}n_{i,\downarrow} = H_U$$

$$H_1 = \sum_{i,j}\sum_{\sigma} t_{i,j}\ (\hat{d}^{\dagger}_{i,\sigma}\hat{c}_{j,\sigma} + \hat{c}^{\dagger}_{i,\sigma}\hat{d}_{j,\sigma}).$$

The requirement on S was

$$H_1 + [S, H_0] = 0 \ \Rightarrow\ H_1 + [S, H_U] = 0$$

We recall the commutator relation for the Hubbard-operators

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

and guess easily (?)

$$S = \sum_{i,j}\sum_{\sigma} \frac{t_{i,j}}{U}\ \left(\ \hat{d}^{\dagger}_{i,\sigma}\hat{c}_{j,\sigma} - \hat{c}^{\dagger}_{i,\sigma}\hat{d}_{j,\sigma}\ \right)$$

$$[S, H_U] = \sum_{i,j}\sum_{\sigma} \frac{t_{i,j}}{U}\ \left(\ [\hat{d}^{\dagger}_{i,\sigma}, H_U]\ \hat{c}_{j,\sigma} - \hat{c}^{\dagger}_{i,\sigma}[\hat{d}_{i,\sigma}, H_U]\ \right)$$

In our application to the Hubbard model we had (remember: $U \gg t_{i,j}$)

$$H_0 = \sum_{i,j}\sum_{\sigma} t_{i,j}\ (\hat{c}^{\dagger}_{i,\sigma}\hat{c}_{j,\sigma} + \hat{d}^{\dagger}_{i,\sigma}\hat{d}_{j,\sigma}) + U\sum_{i} n_{i,\uparrow}n_{i,\downarrow} \approx U\sum_{i} n_{i,\uparrow}n_{i,\downarrow} = H_U$$

$$H_1 = \sum_{i,j}\sum_{\sigma} t_{i,j}\ (\hat{d}^{\dagger}_{i,\sigma}\hat{c}_{j,\sigma} + \hat{c}^{\dagger}_{i,\sigma}\hat{d}_{j,\sigma}).$$

The requirement on S was

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and guess easily (?)

$$S = \sum_{i,j}\sum_{\sigma} \frac{t_{i,j}}{U}\ \left(\ \hat{d}^{\dagger}_{i,\sigma}\hat{c}_{j,\sigma} - \hat{c}^{\dagger}_{i,\sigma}\hat{d}_{j,\sigma}\ \right)$$

$$[S, H_U] = \sum_{i,j}\sum_{\sigma} \frac{t_{i,j}}{U}\ \left(\ -U\ \hat{d}^{\dagger}_{i,\sigma}\ \hat{c}_{j,\sigma} - \hat{c}^{\dagger}_{i,\sigma}U\ \hat{d}_{i,\sigma}\ \right) = -\sum_{i,j}\sum_{\sigma} t_{i,j}\ (\hat{d}^{\dagger}_{i,\sigma}\hat{c}_{j,\sigma} + \hat{c}^{\dagger}_{i,\sigma}\hat{d}_{j,\sigma}) = -H_1$$

We just found

$$S \;=\; \sum_{i,j} \sum_{\sigma} \frac{t_{i,j}}{U} \left(\hat{d}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} - \hat{c}^{\dagger}_{i,\sigma} \hat{d}_{j,\sigma} \right)$$

It follows that $S \propto t_{i,j}/U \ll 1$ so that the truncation of the expansion of H' is justified

$$\begin{aligned} H' \;&=\; H_0 + \frac{1}{2} \left[S, H_1 \right] + \frac{1}{3} \left[S, \left[S, H_1 \right] \right] + \ldots \\ &\approx\; H_0 + \frac{1}{2} \left[S, H_1 \right] \end{aligned}$$

The lowest order correction term then becomes

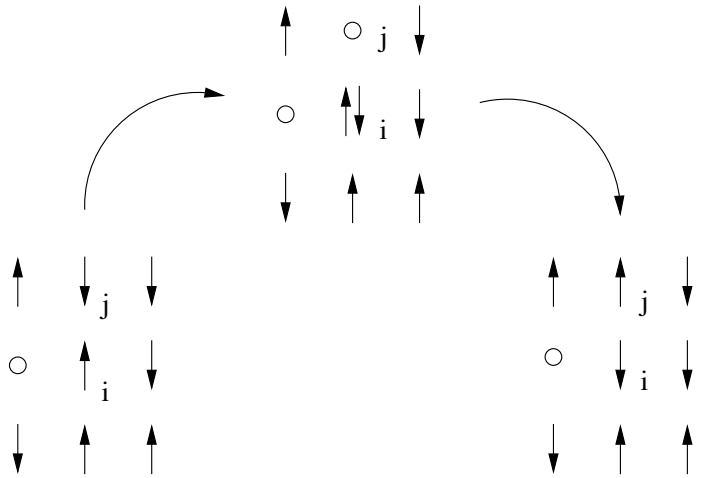
$$\begin{aligned} H'_c = \frac{1}{2} \left[S, H_1 \right] \;&=\; \frac{1}{2} \sum_{i,j,l,m} \sum_{\sigma,\sigma'} \frac{t_{i,j}\, t_{l,m}}{U} \left[\; \hat{d}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} - \hat{c}^{\dagger}_{i,\sigma} \hat{d}_{j,\sigma} \;,\; \hat{d}^{\dagger}_{l,\sigma'} \hat{c}_{m,\sigma'} + \hat{c}^{\dagger}_{l,\sigma'} \hat{d}_{m,\sigma'} \; \right] \\ &=\; -\frac{1}{2} \sum_{i,j,l} \sum_{\sigma,\sigma'} \frac{t_{i,j}\, t_{l,i}}{U} \, \hat{c}^{\dagger}_{l,\sigma'} \hat{d}_{i,\sigma'} \, \hat{d}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} - \frac{1}{2} \sum_{i,j,m} \sum_{\sigma,\sigma'} \frac{t_{i,j}\, t_{j,m}}{U} \, \hat{c}^{\dagger}_{i,\sigma} \hat{d}_{j,\sigma} \, \hat{d}^{\dagger}_{j,\sigma'} \hat{c}_{m,\sigma'} \\ &=\; -\sum_{i,j,l} \sum_{\sigma,\sigma'} \frac{t_{i,l}\, t_{l,j}}{U} \, \hat{c}^{\dagger}_{i,\sigma'} \hat{d}_{l,\sigma'} \, \hat{d}^{\dagger}_{l,\sigma} \hat{c}_{j,\sigma} \end{aligned}$$

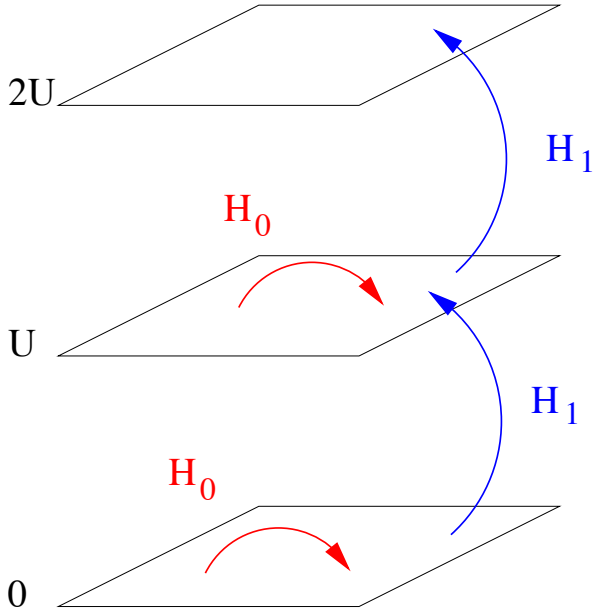
After a straightforward but lengthy calculation we find

$$
\begin{aligned}
H_{sc} \;=\; & \sum_{i,j} \sum_{\sigma} \; t_{i,j} \; \hat{c}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} + \sum_{i,j} \; J_{i,j} \; \left(\; \mathbf{S}_i \cdot \mathbf{S}_j - \frac{n_i n_j}{4} \right) \\
& - \sum_{i,j,l} \; \frac{t_{i,l} \; t_{l,j}}{U} \; \left(\; (\hat{c}^{\dagger}_{i,\downarrow} n_{l,\uparrow} \hat{c}_{j,\downarrow} - \hat{c}^{\dagger}_{i,\uparrow} S^{-}_{l} \, \hat{c}_{j,\downarrow} \;) + (\downarrow \leftrightarrow \uparrow) \; \right)
\end{aligned}
$$

After a straightforward but lengthy calculation we find

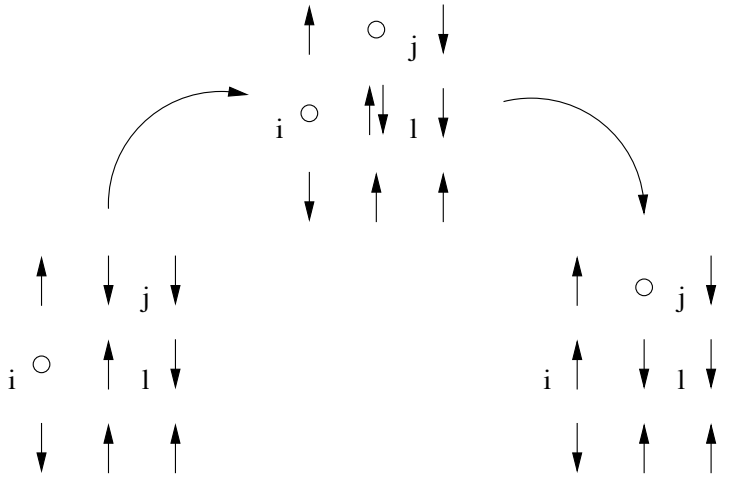
$$H_{sc} = \sum_{i,j}\sum_{\sigma} t_{i,j}\,\hat{c}^{\dagger}_{i,\sigma}\hat{c}_{j,\sigma} + \sum_{i,j} J_{i,j}\left(\left(S^z_i\,S^z_j + \frac{1}{2}\left(S^+_i\,S^-_j + S^-_i\,S^+_j\right)\right) - \frac{n_i n_j}{4}\right)$$
$$- \sum_{i,j,l}\frac{t_{i,l}\,t_{l,j}}{U}\left(\left(\hat{c}^{\dagger}_{i,\downarrow} n_{l,\uparrow}\hat{c}_{j,\downarrow} - \hat{c}^{\dagger}_{i,\uparrow} S^-_l\,\hat{c}_{j,\downarrow}\right) + (\downarrow\leftrightarrow\uparrow)\right)$$

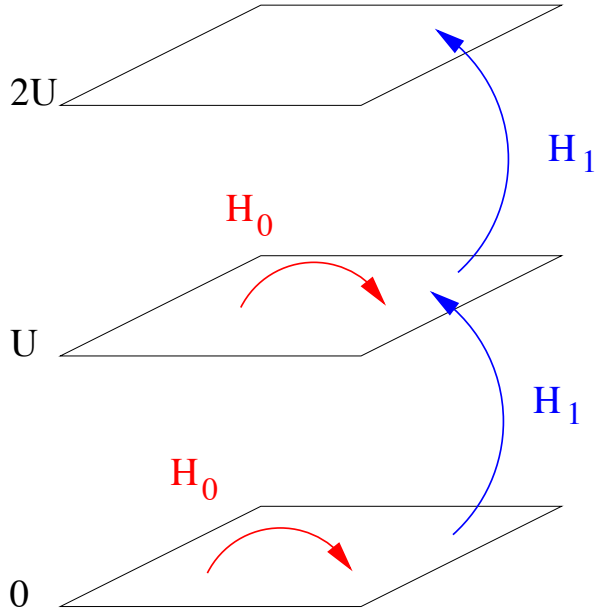




After a straightforward but lengthy calculation we find

$$H_{sc} = \sum_{i,j}\sum_{\sigma} t_{i,j}\,\hat{c}^{\dagger}_{i,\sigma}\hat{c}_{j,\sigma} + \sum_{i,j} J_{i,j}\left(\left(S^z_i\,S^z_j + \frac{1}{2}\left(S^+_i\,S^-_j + S^-_i\,S^+_j\right)\right) - \frac{n_i n_j}{4}\right)$$
$$- \sum_{i,j,l}\frac{t_{i,l}\,t_{l,j}}{U}\left(\left(\hat{c}^{\dagger}_{i,\downarrow} n_{l,\uparrow}\hat{c}_{j,\downarrow} - \hat{c}^{\dagger}_{i,\uparrow} S^-_l\,\hat{c}_{j,\downarrow}\right) + (\downarrow\leftrightarrow\uparrow)\right)$$





Spin waves

The strong coupling Hamiltonian in the sector without double occupancies was

$$H_{sc} = \sum_{i,j}\sum_{\sigma} t_{i,j}\, \hat{c}^{\dagger}_{i,\sigma}\hat{c}_{j,\sigma} + \sum_{i,j} J_{i,j} \left(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{n_i n_j}{4} \right)$$
$$- \sum_{i,j,l} \frac{t_{i,l}\, t_{l,j}}{U} \left((\hat{c}^{\dagger}_{i,\uparrow} n_{l,\downarrow} \hat{c}_{j,\uparrow} - \hat{c}^{\dagger}_{i,\downarrow} S^{+}_{l} \hat{c}_{j,\uparrow}) + (\uparrow \leftrightarrow \downarrow) \right)$$

- We specialize to the case $N_e = N$ - the Mott insulator
- In the sector of the Hilbert space without double occupancies all states have precisely one electron/site
- Every $\hat{c}^{\dagger}_{i,\sigma}$ acting on a state with one electron/site gives zero
- All hopping terms are inoperative
- The Hamiltonian reduces to

$$H_{sc} = \sum_{i,j} J_{i,j} \left(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{n_i n_j}{4} \right)$$

Remember

$$H_{sc} = \sum_{i,j} J_{i,j} \left(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{n_i n_j}{4} \right)$$

Further simplifications:

- $J_{i,j} \neq 0$ only between nearest neighbors
- Drop the term $-J \frac{n_i n_j}{4} \rightarrow -N \cdot \frac{J}{2}$

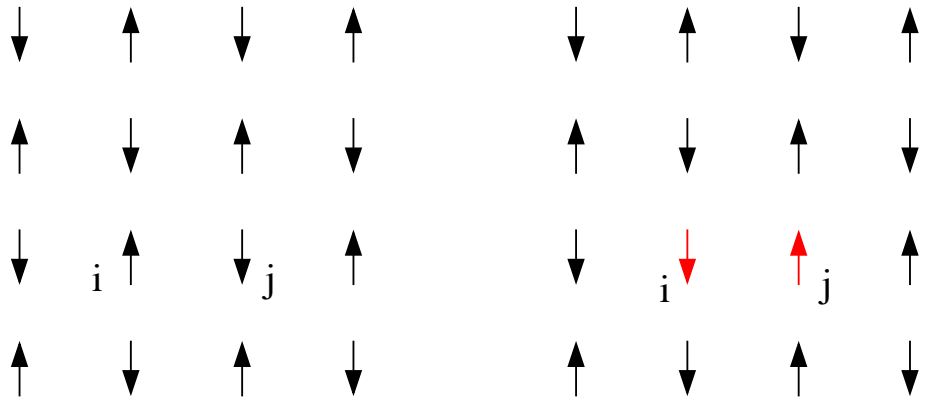
In the end we obtain the Heisenberg antiferromagnet ($\sum_{\langle i,j \rangle}$ denotes sum over nearest neighbor pairs)

$$\begin{aligned} H_{sc} &= J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j \\ &= J \sum_{\langle i,j \rangle} \left(S_i^x \, S_j^x + S_i^y \, S_j^y + S_i^z \, S_j^z \right) \\ &= J \sum_{\langle i,j \rangle} \left(S_i^z \, S_j^z + \frac{1}{2} \left(S_i^+ \, S_j^- + S_i^- \, S_j^+ \right) \right) \end{aligned}$$

The Heisenberg antiferromagnet

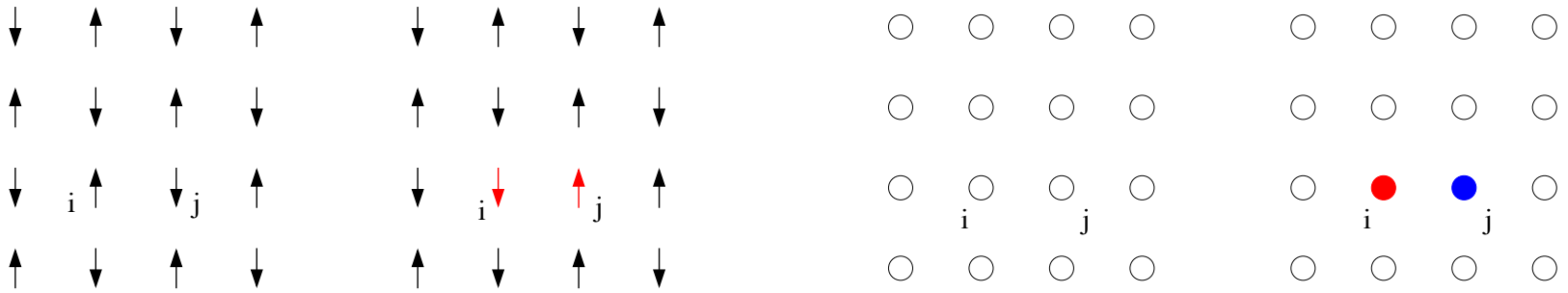
$$H_{sc} = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j = J \sum_{\langle i,j \rangle} \left(S_i^z \, S_j^z + \frac{1}{2} \left(S_i^+ \, S_j^- + S_i^- \, S_j^+ \right) \right)$$

If only the first term were present the ground state would be the Néel state with energy $-2 \cdot N \cdot \frac{J}{4}$



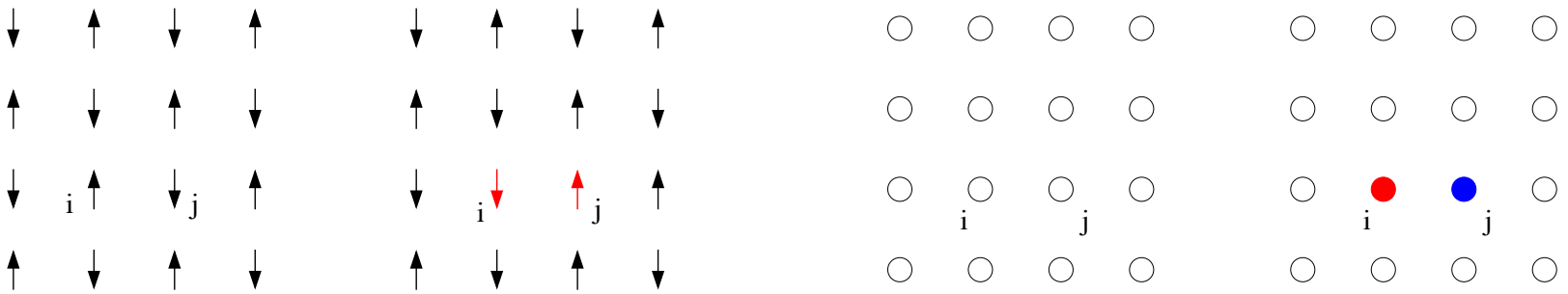
However, the Néel state is not an eigenstate of the full Hamiltonian because the transverse part can produce quantum fluctuations

To deal with the quantum fluctuations we represent the inverted spins as Bosons



- Consider the Néel state as vacuum $|0\rangle$
- Represent an inverted spin at the site i on the $\uparrow$-sublattice as a Boson created by $a_i^\dagger$
- Represent an inverted spin at the site j on the $\downarrow$-sublattice as a Boson created by $b_j^\dagger$
- For example the state on the right would be $a_i^\dagger \; b_j^\dagger \; |0\rangle$
- Why Bosons? - Spin operators on different sites commute!
- States like $(a_i^\dagger)^2|0\rangle$ are meaningless - additional constraint: at most one Boson/site - 'hard core constraint'

Hamiltonian for the Bosons

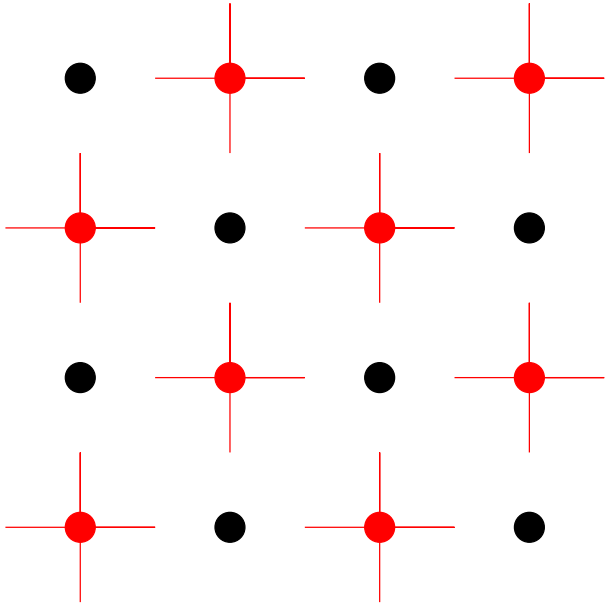


The transverse part creates/annihilates pairs of inverted spins on nearest neighbors

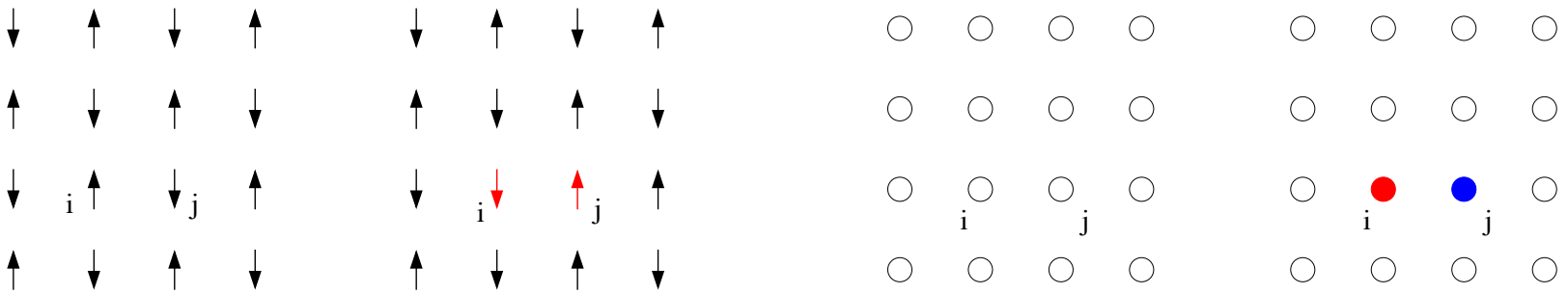
$$J \sum_{\langle i,j \rangle} \frac{1}{2} \left(S_i^- \; S_j^+ + S_i^+ \; S_j^- \right) = \frac{J}{2} \sum_{i \in \uparrow - SL} \sum_{j \in N(i)} \left(S_i^- \; S_j^+ + S_j^- \; S_i^+ \right)$$

$$= \frac{J}{2} \sum_{i \in \uparrow - SL} \sum_{j \in N(i)} \left(a_i^\dagger \quad b_j^\dagger \; + b_j \quad a_i \right)$$

Geometry of the lattice



Hamiltonian for the Bosons



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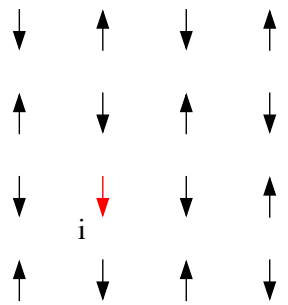
$$J \sum_{\langle i,j \rangle} \frac{1}{2} \left(S_i^- \; S_j^+ + S_i^+ \; S_j^- \right) = \frac{J}{2} \sum_{i \in \uparrow - SL} \sum_{j \in N(i)} \left(S_i^- \; S_j^+ + S_j^- \; S_i^+ \right)$$

$$= \frac{J}{2} \sum_{i \in \uparrow - SL} \sum_{j \in N(i)} \left(a_i^\dagger \quad b_j^\dagger \; + b_j \quad a_i \right)$$

Each inverted spin icreases the expectation value of the term $J \sum_{\langle i,j \rangle} S_i^z \, S_j^z$



- The inverted spin is parallel rather than antiparallel to its $z = 4$ neighbors
- For each bond the energy increases from $-\frac{J}{4}$ to $\frac{J}{4}$
- The total increase of energy is $\frac{zJ}{2}$
- We interpret this as the energy of the boson:

$$J \sum_{\langle i,j \rangle} S_i^z \, S_j^z \; = \; \frac{zJ}{2} \left(\sum_{i \in \uparrow - SL} a_i^\dagger a_i + \sum_{j \in \uparrow - SL} b_j^\dagger b_j \right)$$

In this way we have 'translated' the Hamiltonian of the Heisenberg antiferromagnet into the Boson formulation

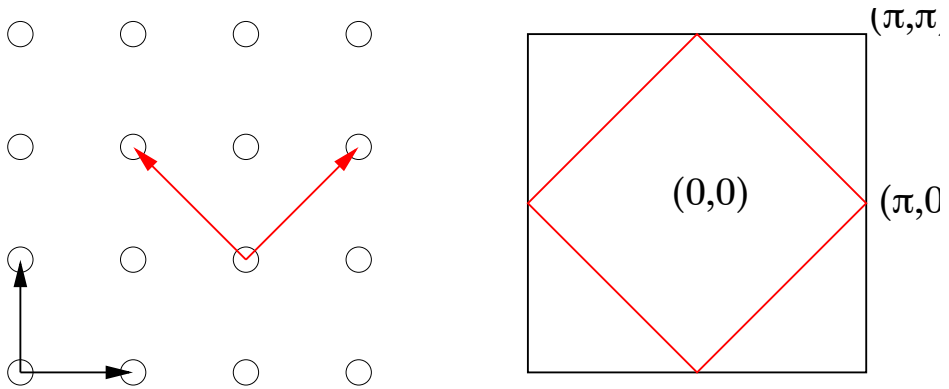
$$H = \frac{zJ}{2}\left(\sum_{i\in\uparrow-SL} a_i^\dagger a_i + \sum_{j\in\uparrow-SL} b_j^\dagger b_j\right) + \frac{J}{2}\sum_{i\in\uparrow-SL}\sum_{j\in N(i)}\left(a_i^\dagger\, b_j^\dagger + b_j\, a_i\right)$$

Fourier transformation yields

$$H_{SW} = \frac{zJ}{2}\sum_{\mathbf{k}}\left(\, a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + b_{\mathbf{k}}^\dagger b_{\mathbf{k}} + \gamma_{\mathbf{k}}\,(a_{\mathbf{k}}^\dagger b_{-\mathbf{k}}^\dagger + b_{-\mathbf{k}} a_{\mathbf{k}})\,\right)$$

$$\gamma_{\mathbf{k}} = \frac{1}{z}\sum_{\mathbf{n}} e^{i\mathbf{k}\cdot\mathbf{n}} = \frac{1}{4}\,(\,2\cos(k_x) + 2\cos(k_y)\,)$$

Thereby $\mathbf{k}$ is a momentum from the antiferromagnetic Brillouin zone:



$$H_{SW} = \frac{zJ}{2} \sum_{\mathbf{k}} \left(a^\dagger_{\mathbf{k}} a_{\mathbf{k}} + b^\dagger_{\mathbf{k}} b_{\mathbf{k}} + \gamma_{\mathbf{k}} \, (a^\dagger_{\mathbf{k}} b^\dagger_{-\mathbf{k}} + b_{-\mathbf{k}} a_{\mathbf{k}}) \right),$$

$$\gamma_{\mathbf{k}} = \frac{1}{z} \sum_{\mathbf{n}} e^{i\mathbf{k}\cdot\mathbf{n}} = \frac{1}{4} (\, 2\cos(k_x) + 2\cos(k_y) \,)$$

This is a quadratic form - but the Bosons have to obey the hard-core constraint of infinite repulsion

However, we now simply ignore the constraint and treat the $a^\dagger$ and $b^\dagger$ as free Bosons

Then H can be diagonalized by a Bosonic Bogoliubov transformation

$$\gamma^\dagger_{a,\mathbf{k}} = u_{\mathbf{k}} \; a^\dagger_{\mathbf{k}} + v_{\mathbf{k}} \, b_{-\mathbf{k}}$$

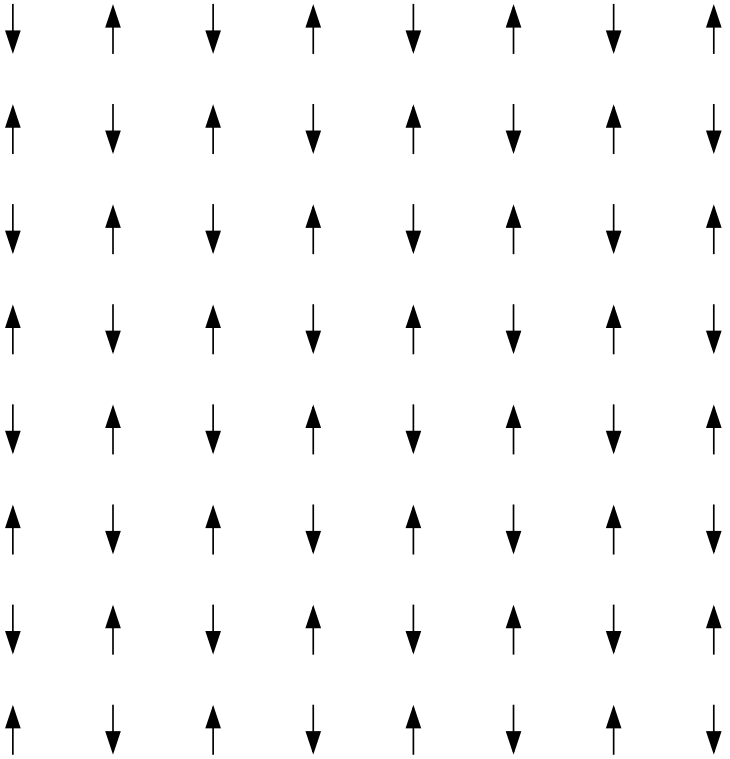
$$\gamma^\dagger_{b,-\mathbf{k}} = u_{\mathbf{k}} \, b^\dagger_{-\mathbf{k}} + v_{\mathbf{k}} \, a_{\mathbf{k}}.$$

Demanding that the magnon operators $\gamma_{a,\mathbf{k}}$ are Bosons: $[\gamma_{a,\mathbf{k}}, \gamma^\dagger_{a,\mathbf{k}}] = 1$, requires $u^2_{\mathbf{k}} - v^2_{\mathbf{k}} = 1$ and demanding $[H, \gamma^\dagger_{a,\mathbf{k}}] = \omega_{\mathbf{k}} \, \gamma^\dagger_{a,\mathbf{k}}$ gives

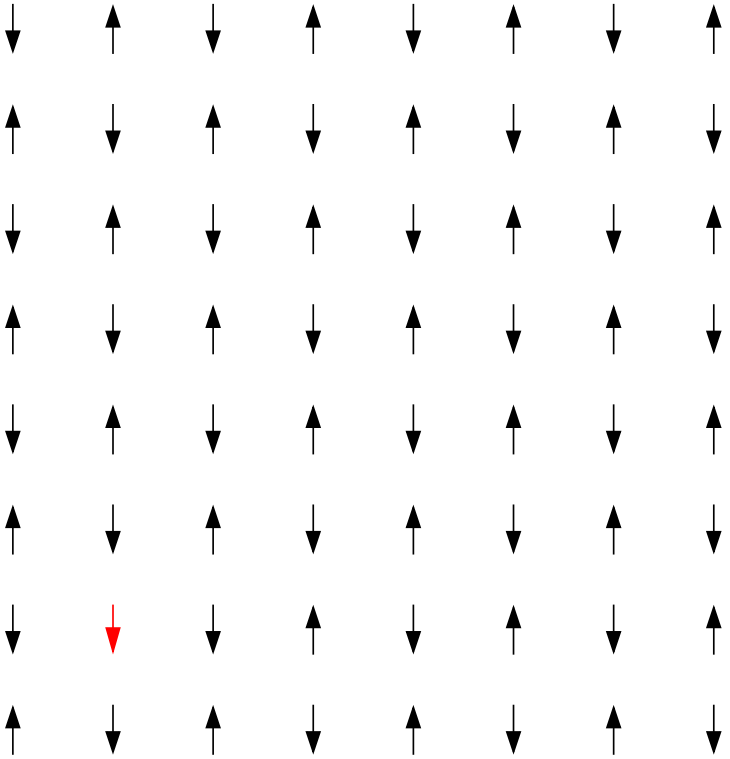
$$\omega_{\mathbf{k}} = \frac{zJ}{2} \sqrt{1 - \gamma^2_{\mathbf{k}}}, \qquad u_{\mathbf{k}} = \sqrt{\frac{1 + \nu_{\mathbf{k}}}{2\nu_{\mathbf{k}}}}, \qquad v_{\mathbf{k}} = \sqrt{\frac{1 - \nu_{\mathbf{k}}}{2\nu_{\mathbf{k}}}}$$

with $\gamma_{\mathbf{k}} = \frac{1}{4} (\, 2\cos(k_x) + 2\cos(k_y) \,)$, $\nu_{\mathbf{k}} = \sqrt{1 - \gamma^2_{\mathbf{k}}}$

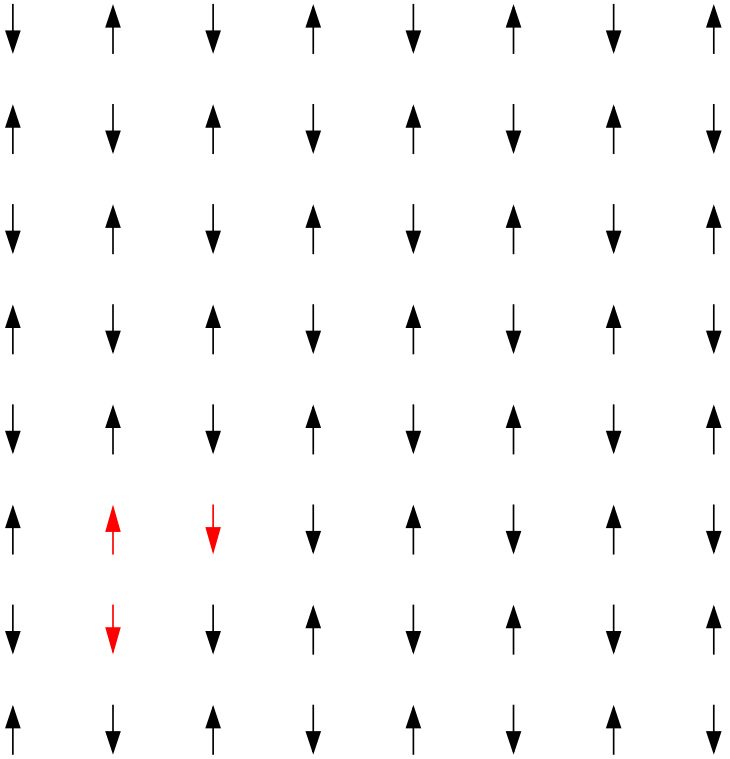
Propagation of a magnon



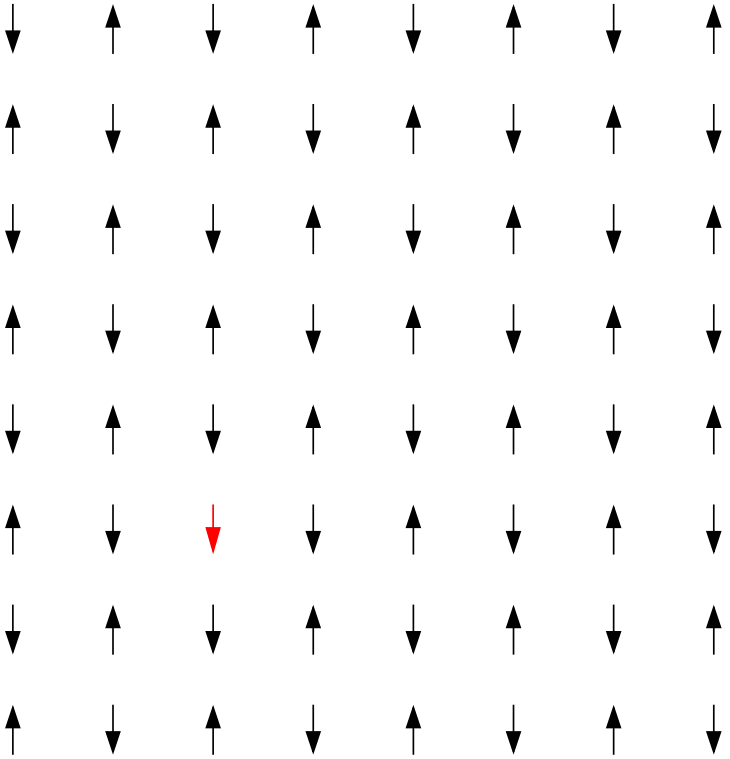
Propagation of a magnon



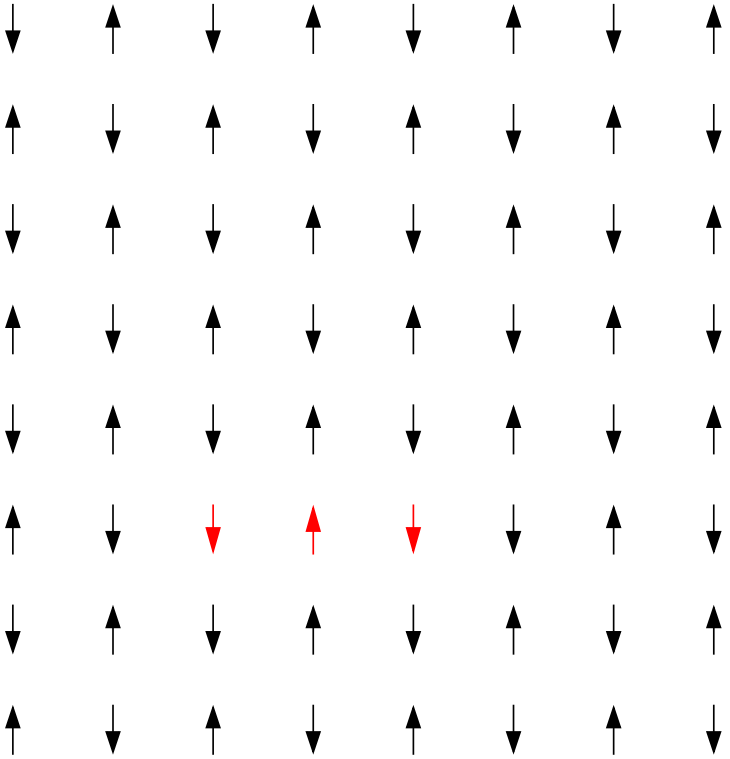
Propagation of a magnon



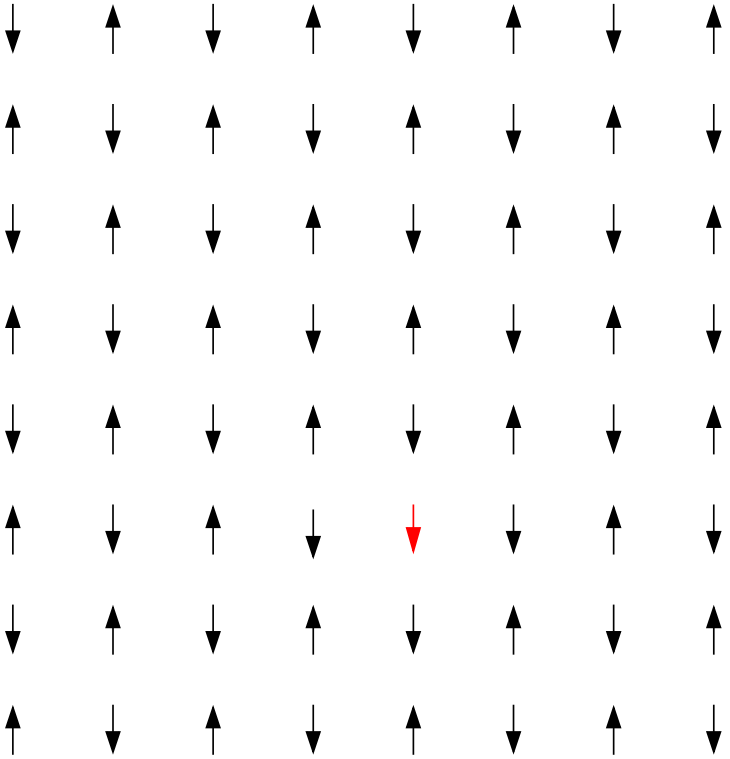
Propagation of a magnon



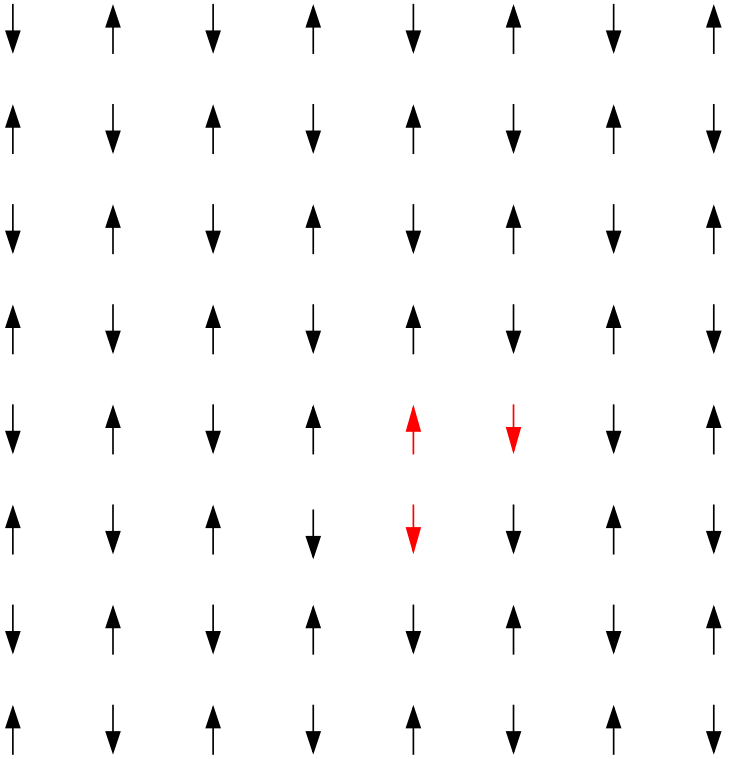
Propagation of a magnon



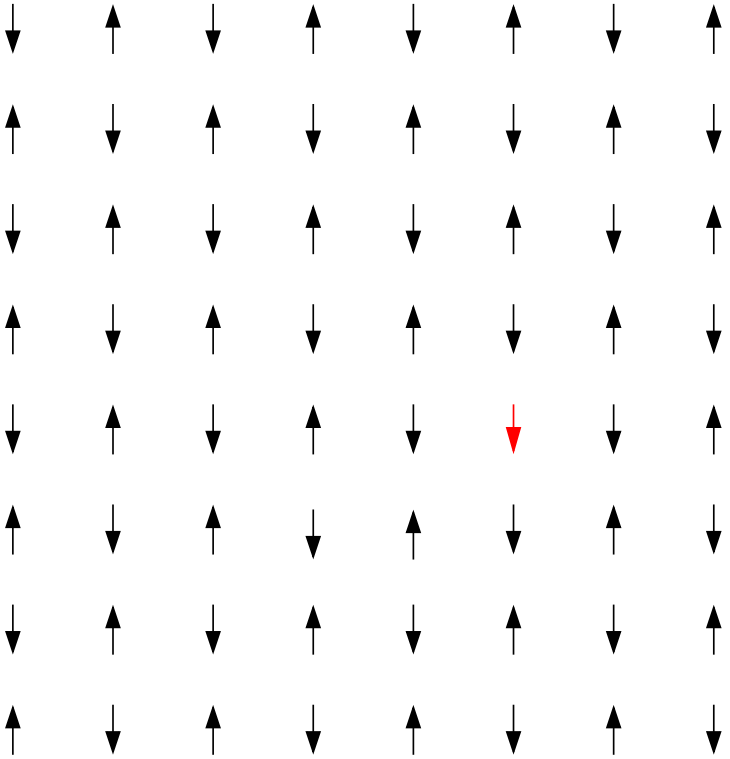
Propagation of a magnon



Propagation of a magnon



Propagation of a magnon



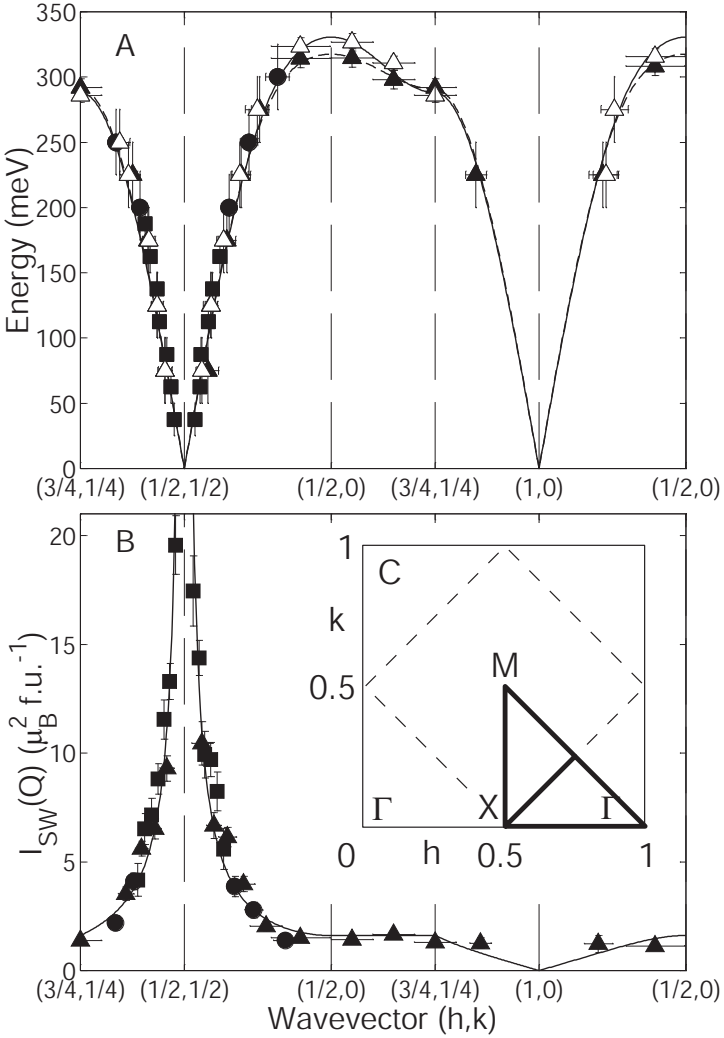
Application: Dispersion and spectral weight of magnons in La_2CuO_4

We had: $\omega_{\mathbf{k}} = \frac{zJ}{2}\sqrt{1-\gamma_{\mathbf{k}}^2}$

$I_{\mathbf{k}} \propto (u_{\mathbf{k}} \pm v_{\mathbf{k}})^2$

Inelastic neutron scattering results from

R. Coldea *et al.*,PRL **86**, 5377 (2001)



Reminder: in our derivation we have simply ignored the hard-core constraint and treated the Bosons as free particles - is this justified? Using the reverse Bogoliubov transformation....

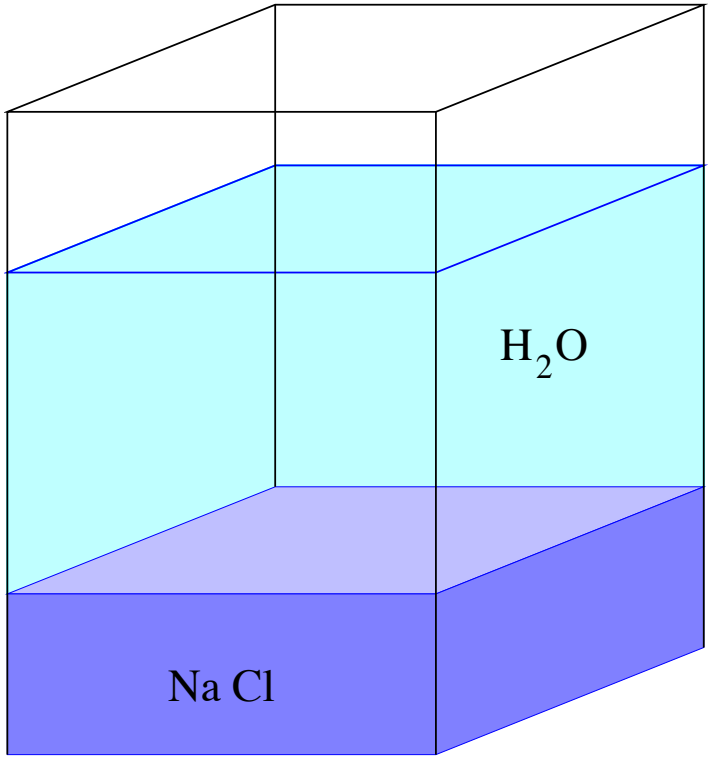
$$\begin{aligned} a_{\mathbf{k}}^{\dagger} &= u_{\mathbf{k}}\, \gamma_{a,\mathbf{k}}^{\dagger} - v_{\mathbf{k}}\, \gamma_{b,-\mathbf{k}} \\ b_{-\mathbf{k}} &= -v_{\mathbf{k}}\, \gamma_{a,\mathbf{k}}^{\dagger} + u_{\mathbf{k}}\, \gamma_{b,-\mathbf{k}} \end{aligned}$$

...we compute the density of a-type Bosons in the ground state $|GS\rangle$ (which obeys $\gamma_{a,\mathbf{k}}|GS\rangle = 0$)

$$\begin{aligned} n_a &= \frac{2}{N} \sum_{\mathbf{k}} \langle GS| a_{\mathbf{k}}^{\dagger}\, a_{\mathbf{k}} |GS\rangle \\ &= \frac{2}{N} \sum_{\mathbf{k}} \langle GS| \left(u_{\mathbf{k}}\, \gamma_{a,\mathbf{k}}^{\dagger} - v_{\mathbf{k}}\, \gamma_{b,-\mathbf{k}}\right) \left(u_{\mathbf{k}}\, \gamma_{a,\mathbf{k}} - v_{\mathbf{k}}\, \gamma_{b,-\mathbf{k}}^{\dagger}\right) |GS\rangle \\ &= \frac{2}{N} \sum_{\mathbf{k}} v_{\mathbf{k}}^2 \end{aligned}$$

- Numerical evaluation for a 2D square lattice gives $n_a = 0.19$
- The probability to have two Bosons on one site would be $\propto n_a^2 = 0.04 \ll 1$
- Enforcing the constraint (e.g. by Gutzwiller projection) would not change much...

Analogy: Equilibrium in a solution



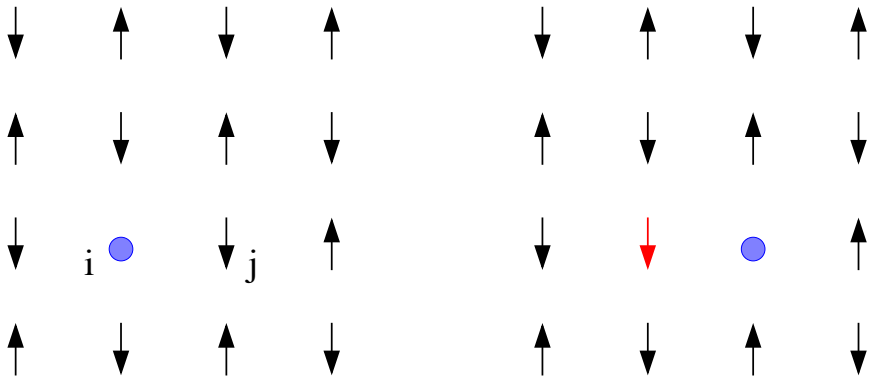
Single hole problem

We return to the strong coupling Hamiltonian:

$$H_{sc} = -t \sum_{\langle i,j \rangle} \sum_{\sigma} \hat{c}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} + J \sum_{\langle i,j \rangle} \left(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{n_i n_j}{4} \right)$$

- We specialize to the case $N_e = N - 1$ - a single hole in the Mott insulator
- For simplicity we discard the three-site hopping terms
- In addition we assume hopping $t_{i,j}$ and exchange $J_{i,j}$ only between nearest neighbors
- The remaining Hamiltonian is called the t-J model

- Basic assumption: a single hole will not destroy antiferromagnetic order
- We continue to use the Néel state as a starting point of the discussion
- Assume that the electron on site $i \in \uparrow -SL$ of the Néel state has been removed



(a) (b)

- The term $-t\ \hat{c}^{\dagger}_{i,\downarrow}\ \hat{c}_{j,\downarrow}$ can transport the hole
- But thereby an inverted spin on site i is left behind
- This is a magnon as introduced in the preceeding discussion
- The hole 'radiates off' magnons as it propagates

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

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

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

The various terms describe

Coherent propagation from $i \to j$

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

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

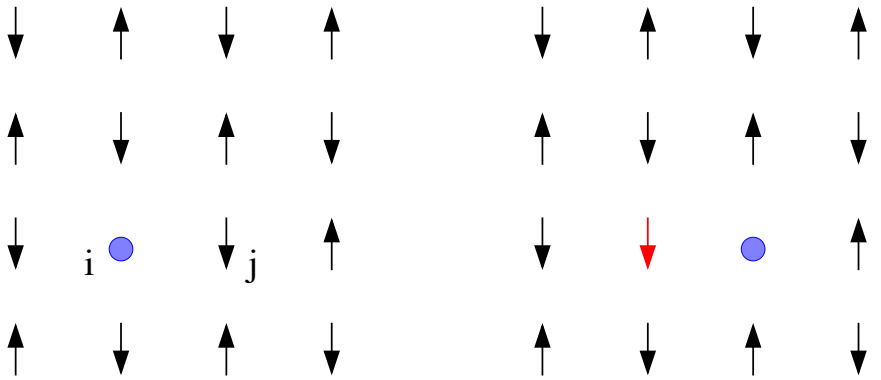
Hopping $i \to j$ while leaving a pair excitation at i (important only for $U < 0$)

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

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

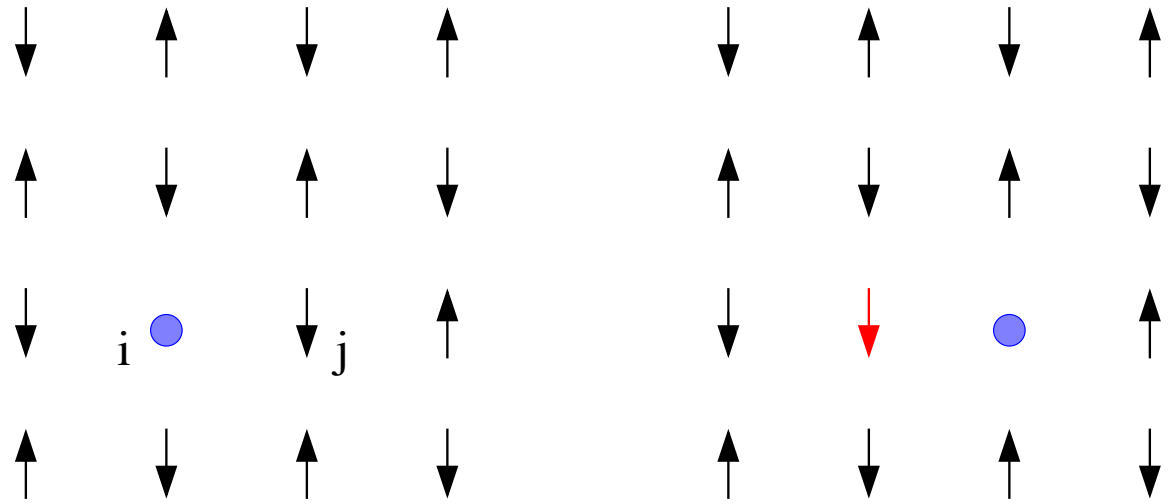
$$[\hat{d}_{i,\uparrow}, H_t] = \sum_j t_{ij} \quad \frac{n_e}{2} \quad c_{j,\uparrow} = \quad \frac{n_e}{2} \quad \sum_j t_{ij} \; (\hat{c}_{j,\uparrow} + \hat{d}_{j,\uparrow})$$

- Basic assumption: a single hole will not destroy antiferromagnetic order
- We continue to use the Néel state as a starting point of the discussion
- Assume that the electron on site $i \in \uparrow -SL$ of the Néel state has been removed



- The term $-t\ \hat{c}^{\dagger}_{i,\uparrow}\ \hat{c}_{j,\uparrow}$ can transport the hole
- But thereby an inverted spin on site i is left behind
- This is a magnon as introduced in the preceeding discussion
- The hole 'radiates off' magnons as it propagates

- We introduce Fermions $h^\dagger_{a,i}$ for $i \in \uparrow$-SL and $h^\dagger_{b,j}$ for $j \in \uparrow$-SL
- we continue to use $a^\dagger_i$ (inverted spin at site $i \in \uparrow$-SL) and $b^\dagger_j$ (inverted spin at site $j \in \downarrow$-SL)



This is described by the Hamiltonian

$$H_{int} = t \sum_{i \in A} \sum_{\mathbf{n}} \left(h^\dagger_{b,i+\mathbf{n}} h_{a,i}\, a^\dagger_i + H.c. \right) + t \sum_{j \in B} \sum_{\mathbf{n}} \left(h^\dagger_{a,j+\mathbf{n}} h_{b,j}\, b^\dagger_j + H.c. \right).$$

We had

$$H_{int} \;=\; t\sum_{i\in A}\sum_{\mathbf{n}}\left(h^{\dagger}_{b,i+\mathbf{n}}h_{a,i}\;a^{\dagger}_{i}+H.c.\right)+t\sum_{j\in B}\sum_{\mathbf{n}}\left(h^{\dagger}_{a,j+\mathbf{n}}h_{b,j}\;b^{\dagger}_{j}+H.c.\right).$$

Fourier transformation gives (with $\epsilon_{\mathbf{k}}=2t(\,\cos(k_x)+\cos(k_y)\,)$)

$$H_{int} \;=\; \sqrt{\frac{2}{N}}\sum_{\mathbf{k},\mathbf{q}}\left(\left(\epsilon_{\mathbf{k}-\mathbf{q}}\;h^{\dagger}_{b,\mathbf{k}-\mathbf{q}}h_{a,\mathbf{k}}\;a^{\dagger}_{\mathbf{q}}+H.c.\right)+(a\leftrightarrow b)\right).$$

Now we recall the Bogoliubov transformation which diagonalized the spin wave Hamiltonian

$$\begin{aligned}\gamma^{\dagger}_{a,\mathbf{k}} &= u_{\mathbf{k}}\;\;a^{\dagger}_{\mathbf{k}}+v_{\mathbf{k}}\;b_{-\mathbf{k}}\\ \gamma^{\dagger}_{b,-\mathbf{k}} &= u_{\mathbf{k}}\;b^{\dagger}_{-\mathbf{k}}+v_{\mathbf{k}}\;a_{\mathbf{k}}.\end{aligned}$$

Replacing $(a^{\dagger}_{\mathbf{k}},b^{\dagger}_{\mathbf{k}})\rightarrow(\gamma^{\dagger}_{a,\mathbf{k}},\gamma^{\dagger}_{b,\mathbf{k}})$ and adding the Hamiltonian for the γ's we finally obtain

$$H_{tot} \;=\; \sqrt{\frac{2}{N}}\sum_{\mathbf{k},\mathbf{q}}\left(\left(M(\mathbf{k},\mathbf{q})\;h^{\dagger}_{b,\mathbf{k}-\mathbf{q}}\;h_{a,\mathbf{k}}\;\gamma^{\dagger}_{a,\mathbf{q}}+H.c.\right)+(a\leftrightarrow b)\right)\;+\;\sum_{\mathbf{q}}\omega_{\mathbf{q}}\left(\gamma^{\dagger}_{a,\mathbf{q}}\gamma_{a,\mathbf{q}}+\gamma^{\dagger}_{b,\mathbf{q}}\gamma_{b,\mathbf{q}}\right)$$

Collecting everything

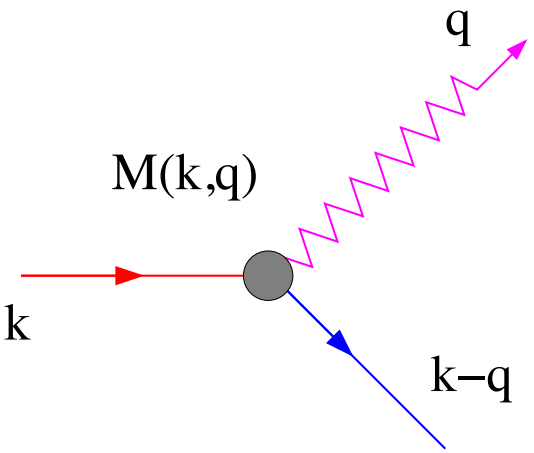
$$H_{tot} = \sqrt{\frac{2}{N}} \sum_{\mathbf{k},\mathbf{q}} \left(\left(M(\mathbf{k},\mathbf{q})\; h^{\dagger}_{b,\mathbf{k}-\mathbf{q}}\; h_{a,\mathbf{k}}\; \gamma^{\dagger}_{a,\mathbf{q}} + H.c. \right) + (a \leftrightarrow b) \right) + \sum_{\mathbf{q}} \omega_{\mathbf{q}} \left(\gamma^{\dagger}_{a,\mathbf{q}} \gamma_{a,\mathbf{q}} + \gamma^{\dagger}_{b,\mathbf{q}} \gamma_{b,\mathbf{q}} \right)$$

- $M(\mathbf{k},\mathbf{q}) = \epsilon_{\mathbf{k}-\mathbf{q}}\; u_{\mathbf{q}} - \epsilon_{\mathbf{k}}\; v_{\mathbf{q}}$
- $\epsilon_{\mathbf{k}} = 2t\; (\; \cos(k_x) + \cos(k_y)\;)$

$$\gamma^{\dagger}_{a,\mathbf{k}} = u_{\mathbf{k}}\; a^{\dagger}_{\mathbf{k}} + v_{\mathbf{k}}\; b_{-\mathbf{k}}$$
$$\gamma^{\dagger}_{b,-\mathbf{k}} = u_{\mathbf{k}}\; b^{\dagger}_{-\mathbf{k}} + v_{\mathbf{k}}\; a_{\mathbf{k}}.$$

- $\omega_{\mathbf{q}} = \frac{zJ}{2} \sqrt{1 - \gamma^2_{\mathbf{q}}}$
- $\gamma_{\mathbf{k}} = \frac{1}{z} \sum_{\mathbf{n}} e^{i\mathbf{k}\cdot\mathbf{n}} = \frac{1}{4}\; (\; 2\cos(k_x) + 2\cos(k_y)\;)$

$M(\mathbf{k},\mathbf{q})\; h^{\dagger}_{b,\mathbf{k}-\mathbf{q}}\; h_{a,\mathbf{k}}\; \gamma^{\dagger}_{a,\mathbf{q}}$



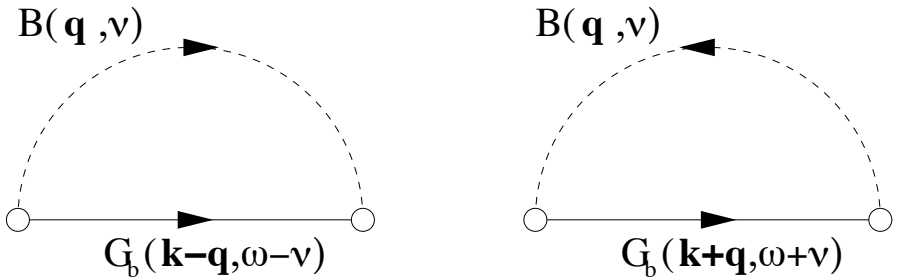
We have to use an approximation - widely used is the self-consistent Born approximation (SCBA)

This assumes that the self-energy for the holes is given in terms of the simplest diagrams possible

Define time ordered Green's functions ($\langle \dots \rangle$: expectation value in the state with no hole and no magnons)

$$
\begin{aligned}
G_\alpha(\mathbf{k},t) &= -i\langle T\; h_{\alpha,\mathbf{k}}(t) h^\dagger_{\alpha,\mathbf{k}}(0)\rangle \\
B_\alpha(\mathbf{q},t) &= -i\langle T\; \gamma_{\alpha,\mathbf{q}}(t) \gamma^\dagger_{,\alpha,\mathbf{q}}(0)\rangle,
\end{aligned}
$$

Diagrams for the self-energy



$$
\Sigma_a(\mathbf{k},\omega) = \frac{i}{2\pi}\frac{2}{N}\sum_{\mathbf{q}}\int d\nu\; [\; M^2(\mathbf{k},\mathbf{q})\; B_a(\mathbf{q},\nu)\; G_b(\mathbf{k}-\mathbf{q},\omega-\nu) + M^2(\mathbf{k}+\mathbf{q},\mathbf{q})\; B_a(\mathbf{q},\nu)\; G_b(\mathbf{k}+\mathbf{q},\omega+\nu)\;]
$$

We had

$$\Sigma_a(\mathbf{k},\omega) \;=\; \frac{i}{2\pi}\,\frac{2}{N}\sum_{\mathbf{q}}\int d\nu\;[\;M^2(\mathbf{k},\mathbf{q})\;B_a(\mathbf{q},\nu)G_b(\mathbf{k}-\mathbf{q},\omega-\nu)+M^2(\mathbf{k}+\mathbf{q},\mathbf{q})\;B_a(\mathbf{q},\nu)G_b(\mathbf{k}+\mathbf{q},\omega+\nu)\;]$$

Since we consider only a single hole in an infinite system we can replace the magnon Green's function by that of the system without a hole i.e. the Heisenberg antiferromagnet (whereby $\langle\ldots\rangle$: expectation value in the state with no hole and no magnons)

$$B^{(0)}_\alpha(\mathbf{q},t) \;=\; -ie^{-i\omega_{\mathbf{q}}t}\left(\;\Theta(t)\;\;\langle\gamma_{\alpha,\mathbf{q}}\gamma^\dagger_{\alpha,\mathbf{q}}\rangle+\Theta(-t)\;\;\langle\gamma^\dagger_{\alpha,\mathbf{q}}\gamma_{\alpha,\mathbf{q}}\rangle\;\right)=-i\Theta(t)\;e^{-i\omega_{\mathbf{q}}t},$$

with Fourier transform

$$B^{(0)}_\alpha(\mathbf{q},\omega)=\frac{1}{\omega-\omega_{\mathbf{q}}+i0^+}$$

so that

$$\Sigma_a(\mathbf{k},\omega) \;=\; \frac{i}{2\pi}\,\frac{2}{N}\sum_{\mathbf{q}}\int\;d\nu\;\left[\;M^2(\mathbf{k},\mathbf{q})\;\frac{G_b(\mathbf{k}-\mathbf{q},\omega-\nu)}{\nu-\omega_{\mathbf{q}}+i0^+}+M^2(\mathbf{k}+\mathbf{q},\mathbf{q})\;\frac{G_b(\mathbf{k}+\mathbf{q},\omega+\nu)}{\nu-\omega_{\mathbf{q}}+i0^+}\;\right].$$

Short digression: The Hamiltonian was

$$H \;=\; \sqrt{\frac{2}{N}} \sum_{\mathbf{k},\mathbf{q}} \Big(\Big(M(\mathbf{k},\mathbf{q})\; h^{\dagger}_{b,\mathbf{k}-\mathbf{q}}\; h_{a,\mathbf{k}}\; \gamma^{\dagger}_{a,\mathbf{q}} + H.c. \Big) + (a \leftrightarrow b) \Big) \;+\; \sum_{\mathbf{q}} \omega_{\mathbf{q}} \; \Big(\gamma^{\dagger}_{a,\mathbf{q}} \gamma_{a,\mathbf{q}} + \gamma^{\dagger}_{b,\mathbf{q}} \gamma_{b,\mathbf{q}} \Big)$$

$\rightarrow$ The hole Green's function is ($\alpha \in a, b$)

$$G_{\alpha}(\mathbf{q},t) \;=\; -i \left(\Theta(t) \;\langle\, e^{iHt}\; h_{\alpha,\mathbf{q}}\; e^{-iHt}\; h^{\dagger}_{\alpha,\mathbf{q}} \,\rangle - \Theta(-t) \;\langle\, h^{\dagger}_{\alpha,\mathbf{q}}\; e^{iHt}\; h_{\alpha,\mathbf{q}}\; e^{-iHt} \,\rangle \right)$$

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It follows that

$$G_{\alpha}(\mathbf{q},\omega) \;=\; \int_0^{\infty} dt\; e^{i\omega t}\; G_{\alpha}(\mathbf{q},t)$$

is analytic in the upper ω-half plane: Let

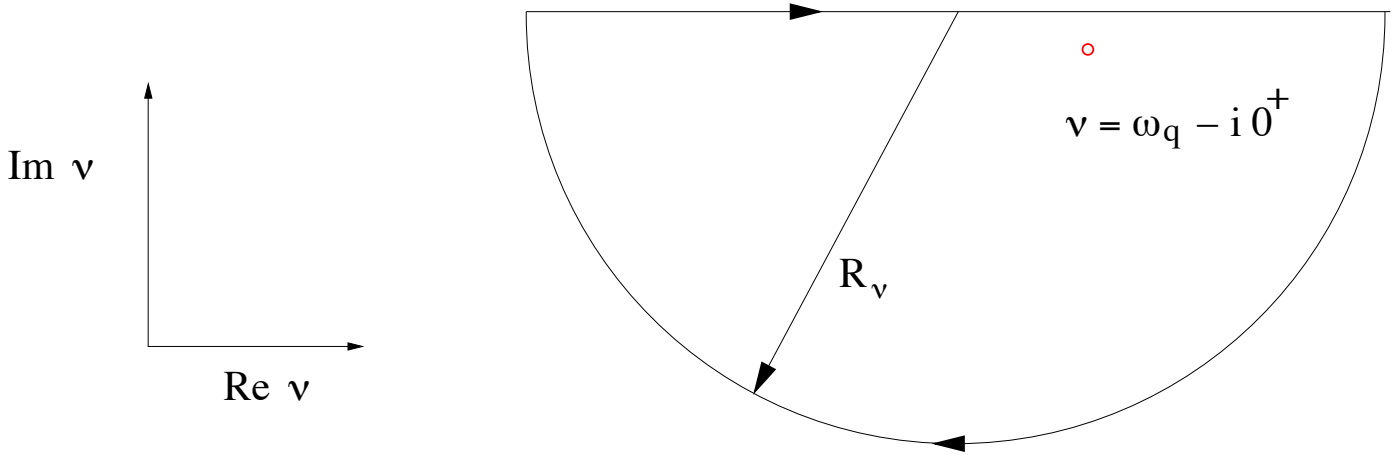
$$\omega = \omega' + i\omega'' \Rightarrow e^{i\omega t} = e^{i\omega' t}\; e^{-\omega'' t}$$

$\Rightarrow$ The hole Green's function $G_{\alpha}(\mathbf{q},\omega)$ is analytic in the upper ω half-plane

Now we can perform the integral over ν

$$\Sigma_a(\mathbf{k},\omega) \;=\; \frac{i}{2\pi}\,\frac{2}{N}\sum_{\mathbf{q}}\int_{\infty}^{\infty} d\nu\;\left[\, M^2(\mathbf{k},\mathbf{q})\,\frac{G_b(\mathbf{k}-\mathbf{q},\omega-\nu)}{\nu-\omega_{\mathbf{q}}+i0^+} + M^2(\mathbf{k}+\mathbf{q},\mathbf{q})\,\frac{G_b(\mathbf{k}+\mathbf{q},\omega+\nu)}{\nu-\omega_{\mathbf{q}}+i0^+}\,\right]$$

- Since $G(\nu)\to\frac{1}{\nu}$ the integrand behaves like $\frac{1}{\nu^2}$
- To perform the integral over ν we may therefore close the contour by a large semi-arc
- For the first term we choose the lower arc



$$\Sigma_a(\mathbf{k},\omega) \;=\; (-2\pi i)\,\frac{i}{2\pi}\,\frac{2}{N}\sum_{\mathbf{q}}\; M^2(\mathbf{k},\mathbf{q})\;G_b(\mathbf{k}-\mathbf{q},\omega-\omega_{\mathbf{q}})$$

We had

$$\Sigma_a(\mathbf{k},\omega) \;=\; \frac{2}{N}\sum_{\mathbf{q}} M^2(\mathbf{k},\mathbf{q})\; G_b(\mathbf{k}-\mathbf{q},\omega-\omega_{\mathbf{q}})$$

and

$$G_a(\mathbf{k},\omega) \;=\; \frac{1}{\omega-\Sigma_a(\mathbf{k},\omega)}$$

Since $G_a = G_b = G$ and $\Sigma_a = \Sigma_b = \Sigma$ we obtain

$$\Sigma(\mathbf{k},\omega) \;=\; \frac{2}{N}\sum_{\mathbf{q}} \frac{M^2(\mathbf{k},\mathbf{q})}{\omega-\omega_{\mathbf{q}}-\Sigma(\mathbf{k}-\mathbf{q},\omega-\omega_{\mathbf{q}})}$$

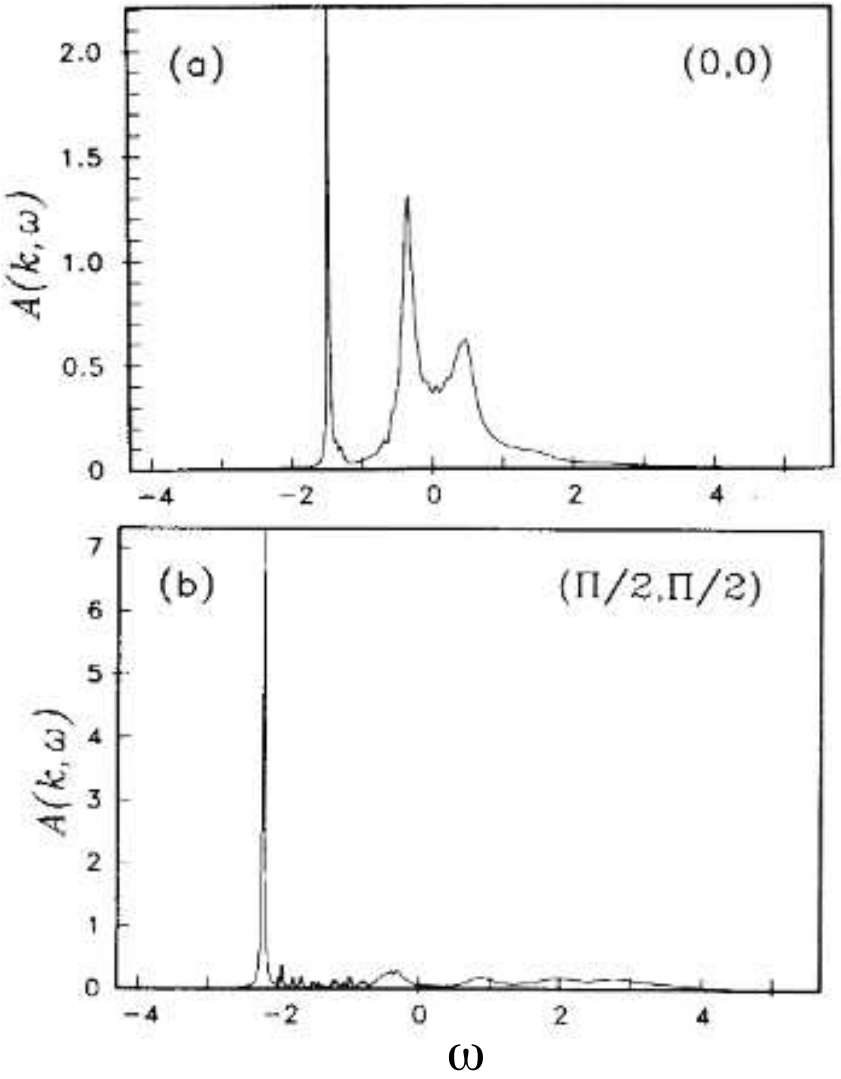
With

- $M(\mathbf{k},\mathbf{q}) = \epsilon_{\mathbf{k}-\mathbf{q}}\, u_{\mathbf{q}} - \epsilon_{\mathbf{k}}\, v_{\mathbf{q}}$
- $\omega_{\mathbf{q}} = \frac{zJ}{2}\sqrt{1-\gamma_{\mathbf{q}}^2}$

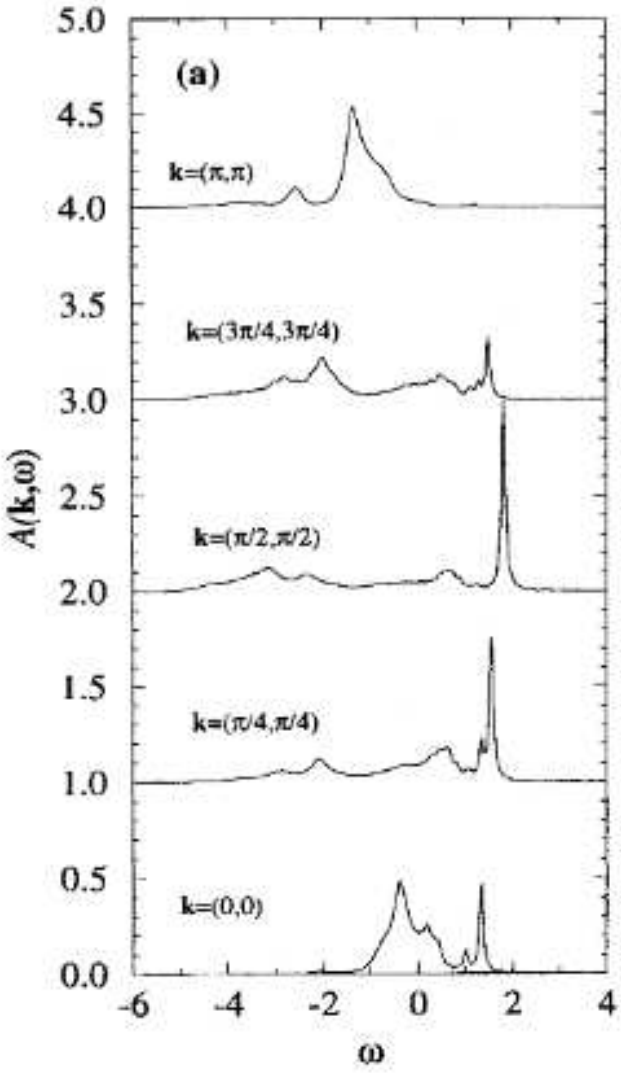
This is a self-consistency equation for $\Sigma(\mathbf{k},\omega)$ which has to be solved numerically for a discrete $\mathbf{k}$- and ω-mesh

Outcome of such a calculation (G. Martinez and P. Horsch, PRB 44, 317 (1991))

compared Lanczos on a 32-site cluster (P.W. Leung and R.J. Gooding PRB $\mathbf{52}$, R15711 (1995))

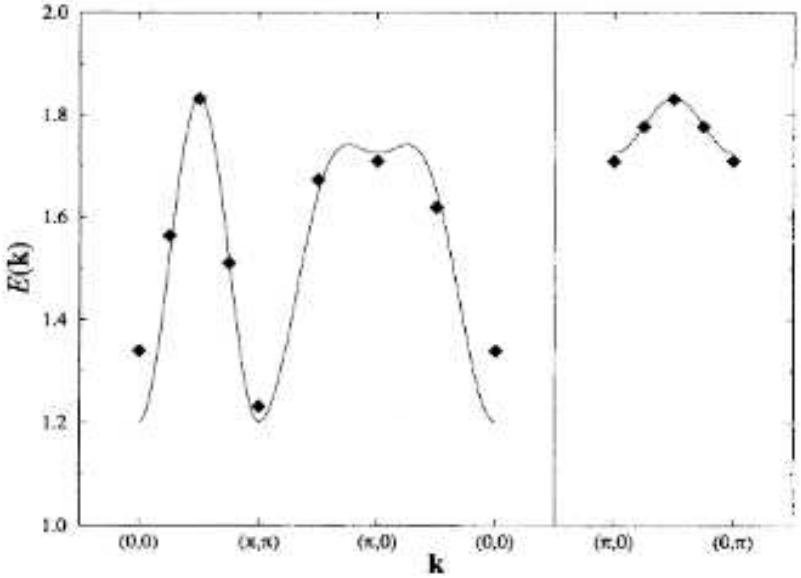


(a)

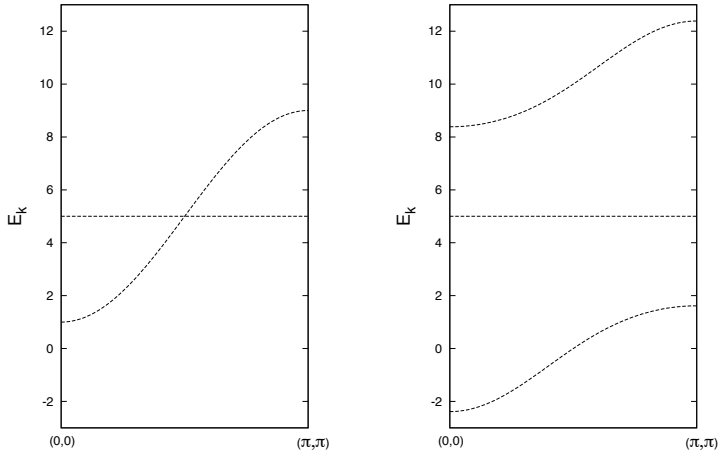


(b)

Dispersion of the 'quasiparticle peak' from the SCBA compared to Lanczos

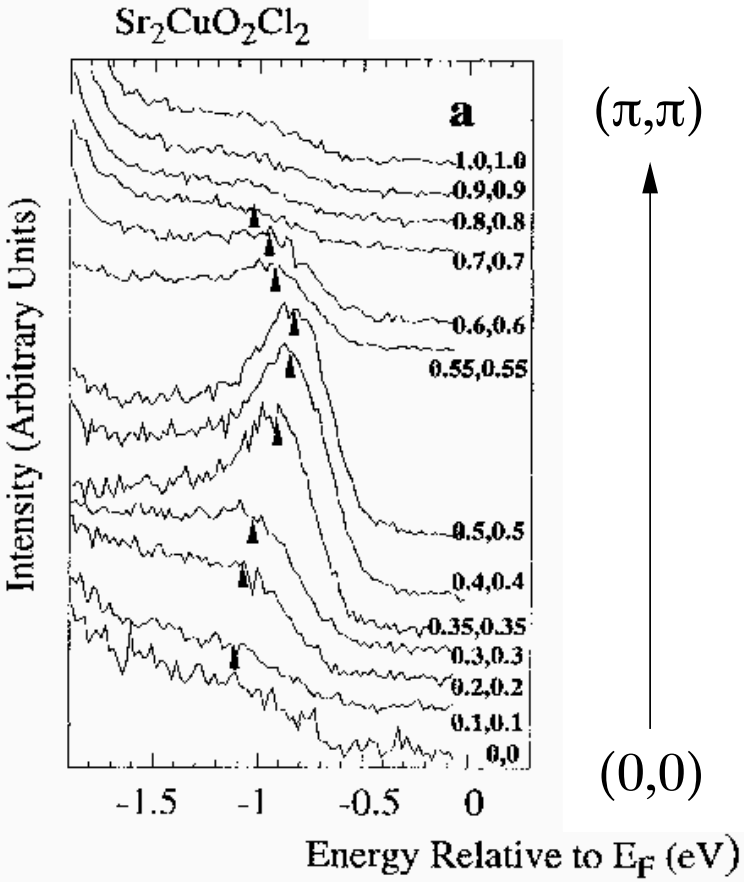


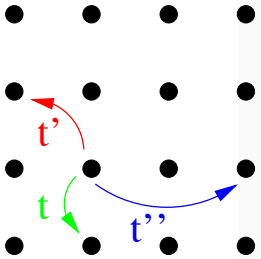
Hubbard-I:



- Width of lower Hubbard band $4t \rightarrow 0.6t$ - actually the bandwidth is $\propto J$
- Change of dispersion - maximum shifted $(\pi, \pi) \rightarrow (\frac{\pi}{2}, \frac{\pi}{2})$
- Bulk of spectral weight shifted to incoherent continua
- All in all: massive change of the photoemission spectrum

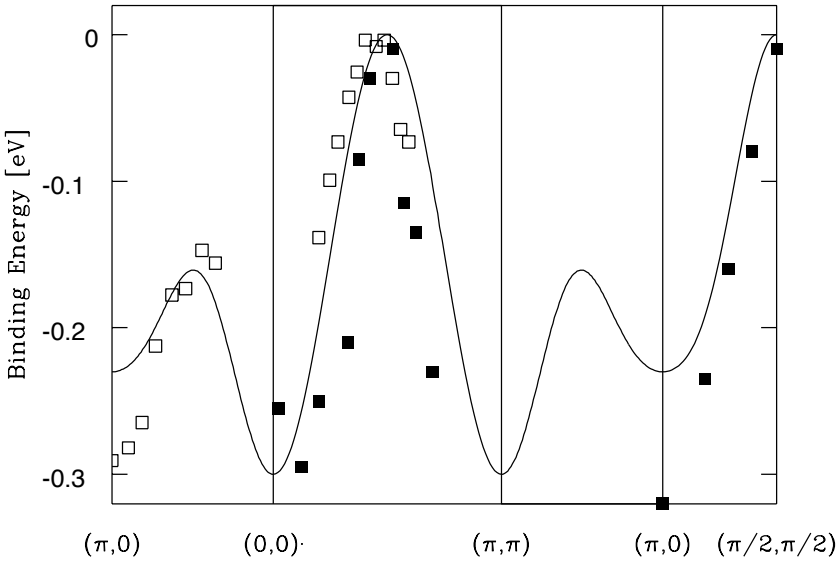
Comparison with experiment: ARPES spectra for $Sr_2CuO_2Cl_2$ (B. O. Wells *et al.*, PRL **74**, 964 (1995))





By adding t' and t'' one can obtain good agreement

(O. Sushkov *et al.*, PRB, **56**, 11769 (1997))



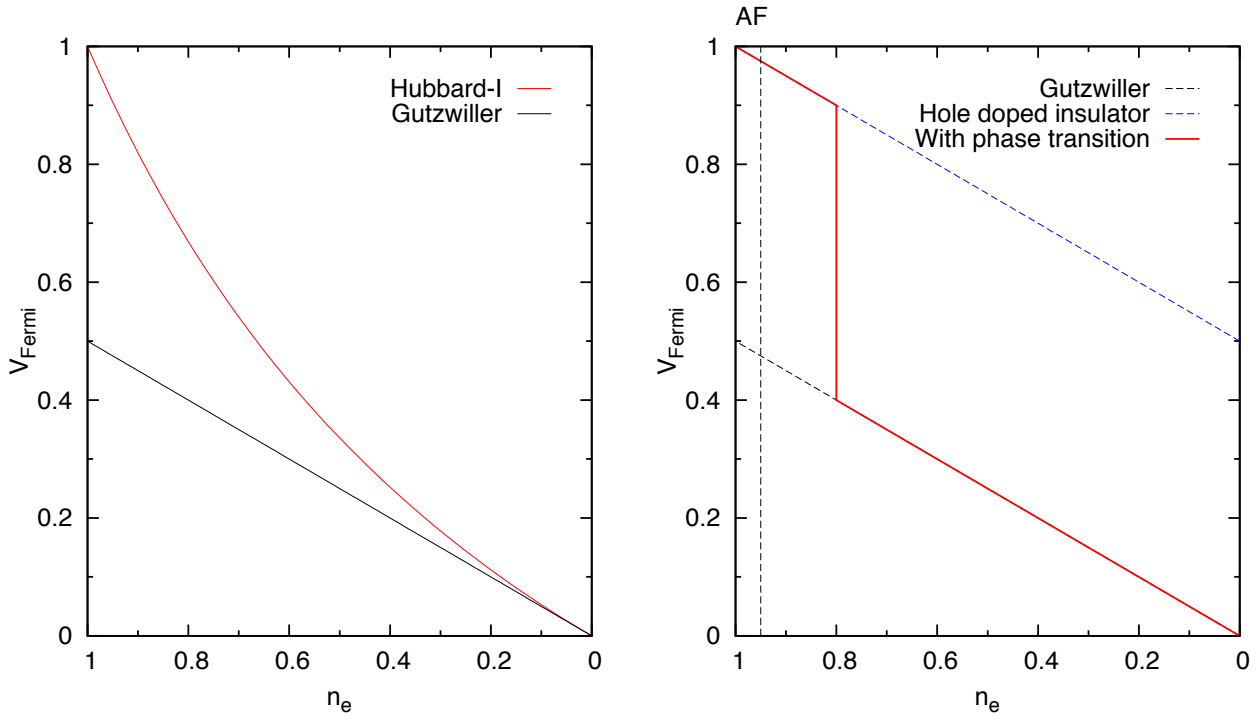
ARPES Data by B. O. Wells *et al.*, Phys. Rev. Lett. **74**, 964 (1995)

Summary: Problems to be solved

- A first major problem: what is the Fermi surface of a lightly doped Mott insulator? Hubbard-I vs. Gutzwiller?
- The 'holes' have strong coupling to collective modes - even for the simplified case of a single hole a very involved calculation was necessary leading to strong modification of the 'band structure'
- A few percent of holes destroys antiferromagnetic order - we have no theory for the spin excitations of such a disordered state that would be a simple and accurate as spin wave theory

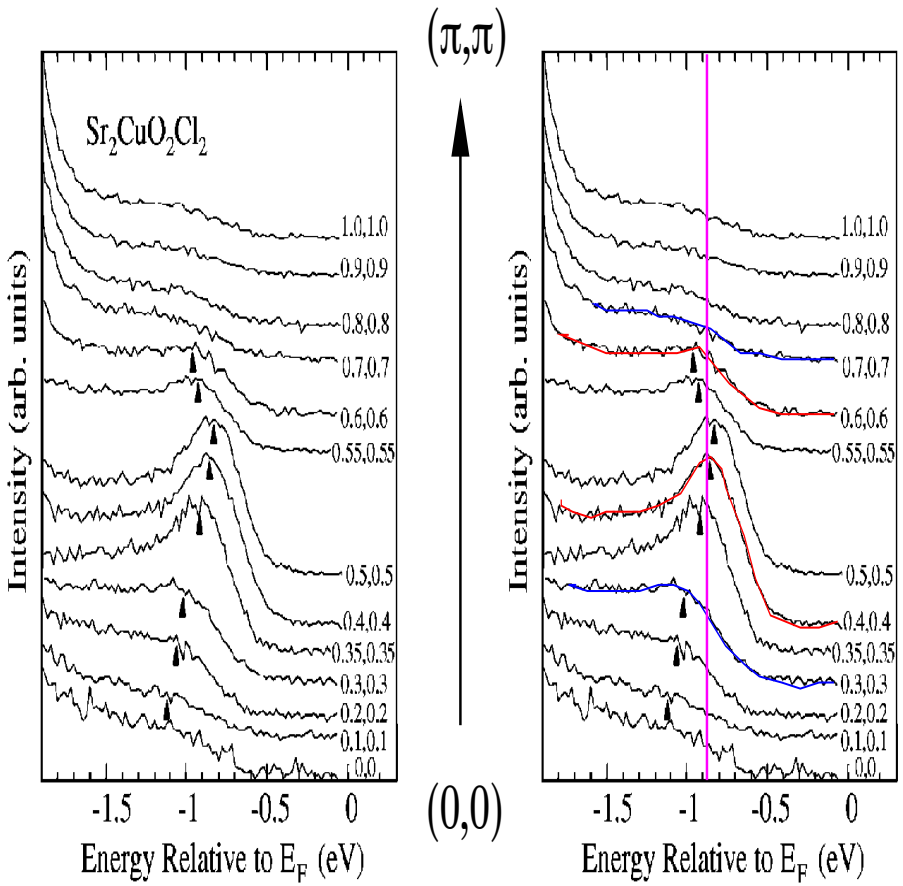
Possible Scenario

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?

Does one see anything like this in experiment?



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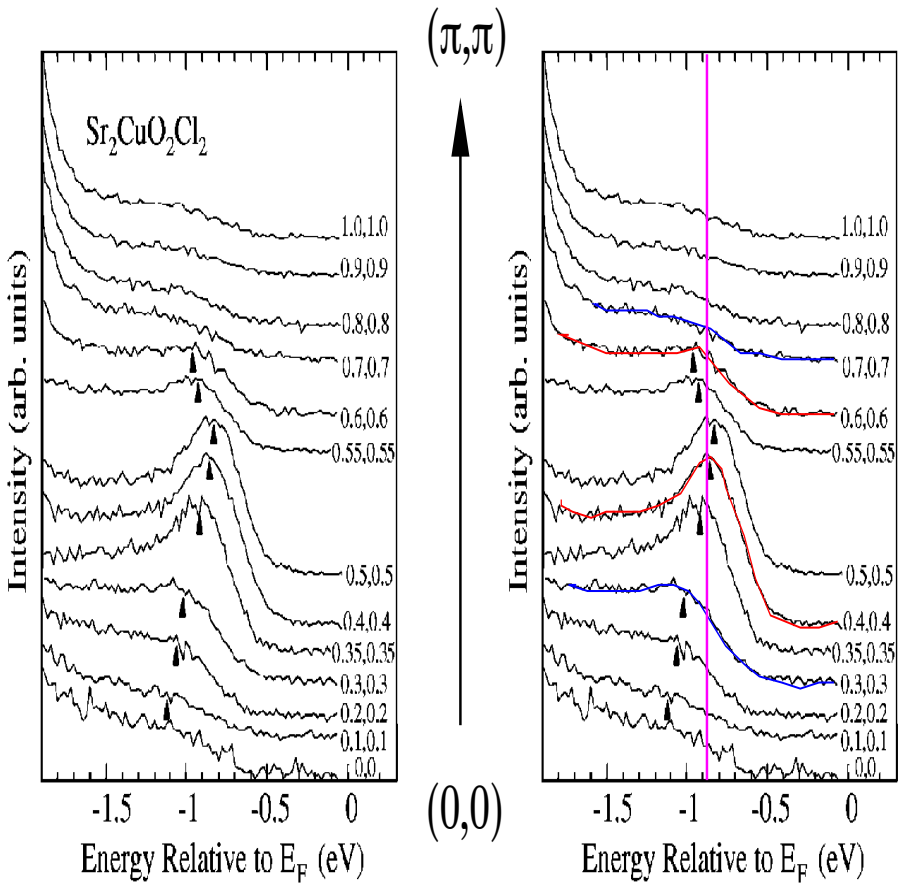
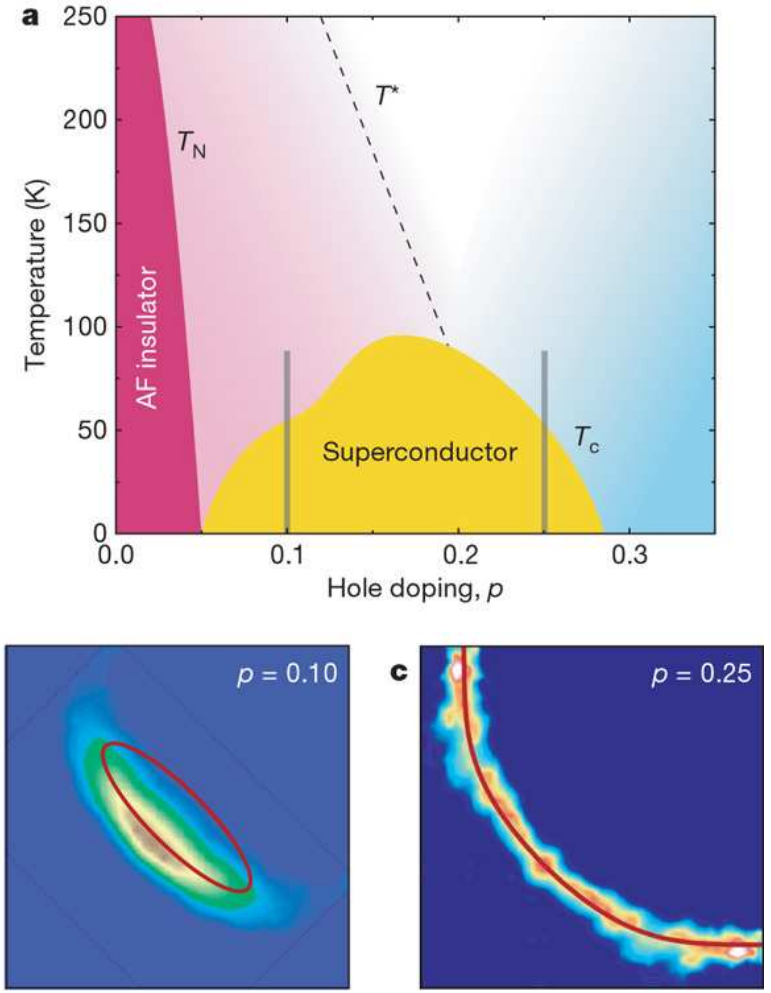
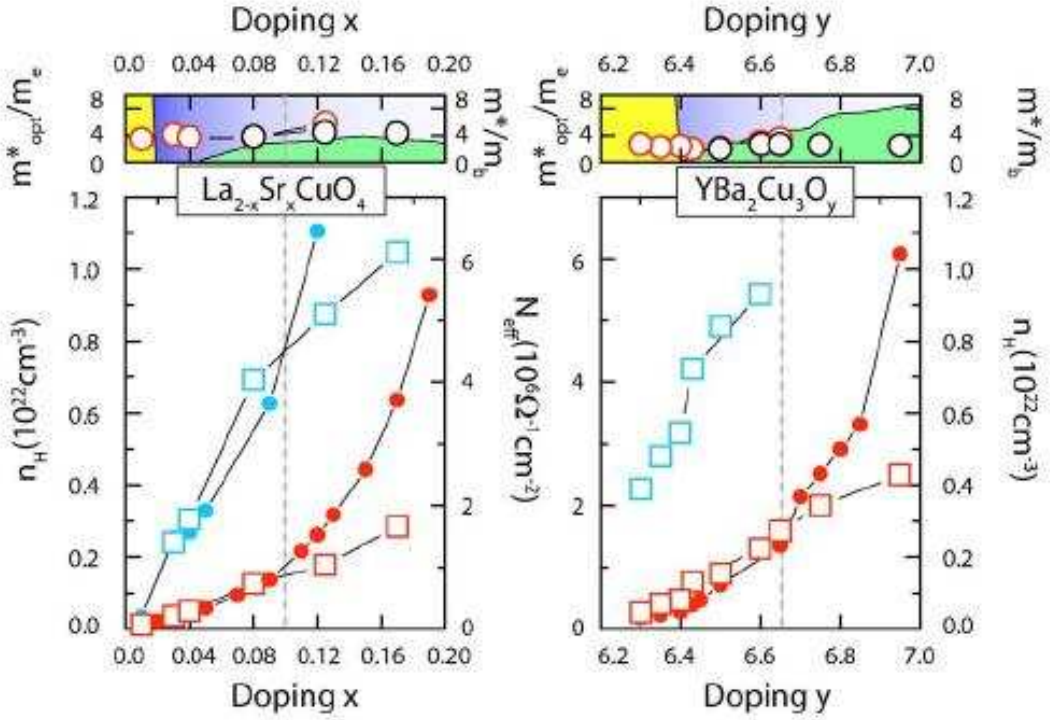
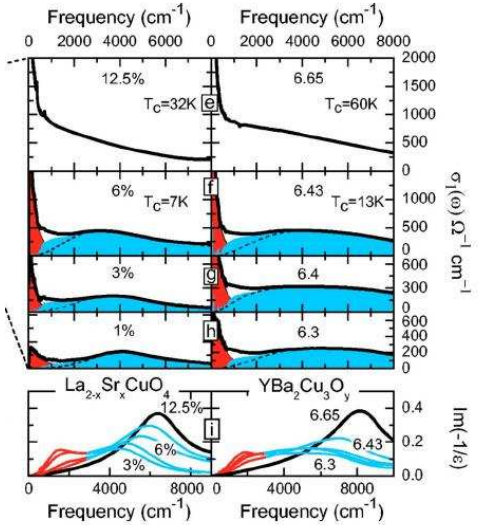




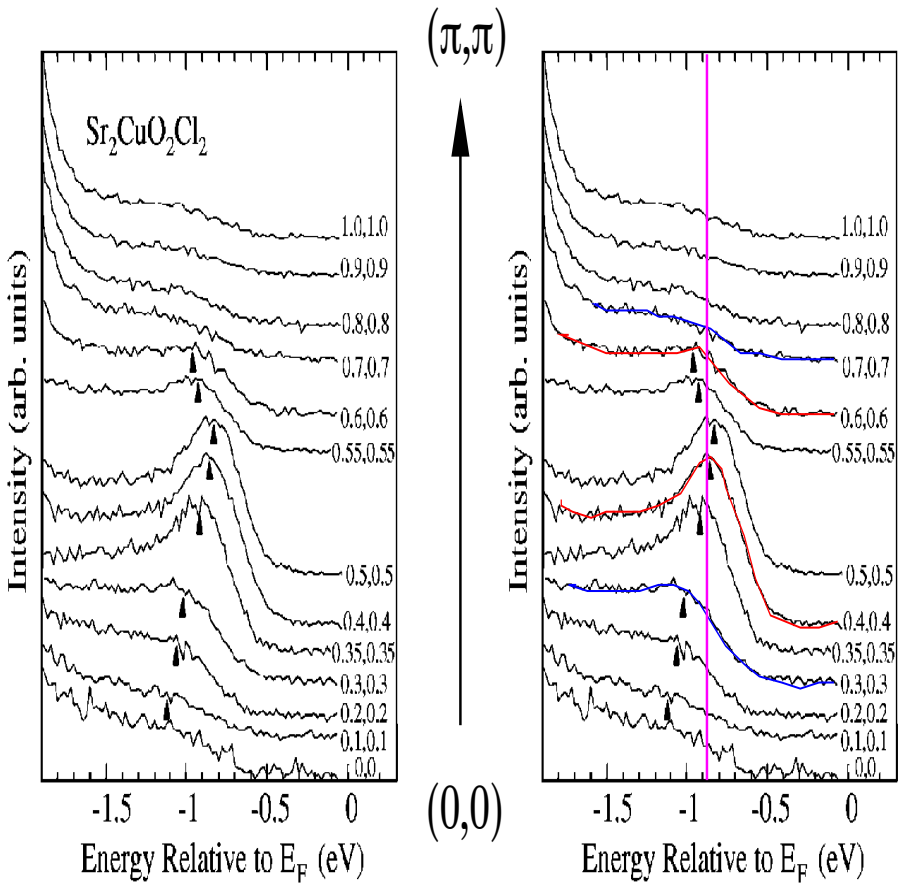
Transport properties also are consistent with a 'small' Fermi surface

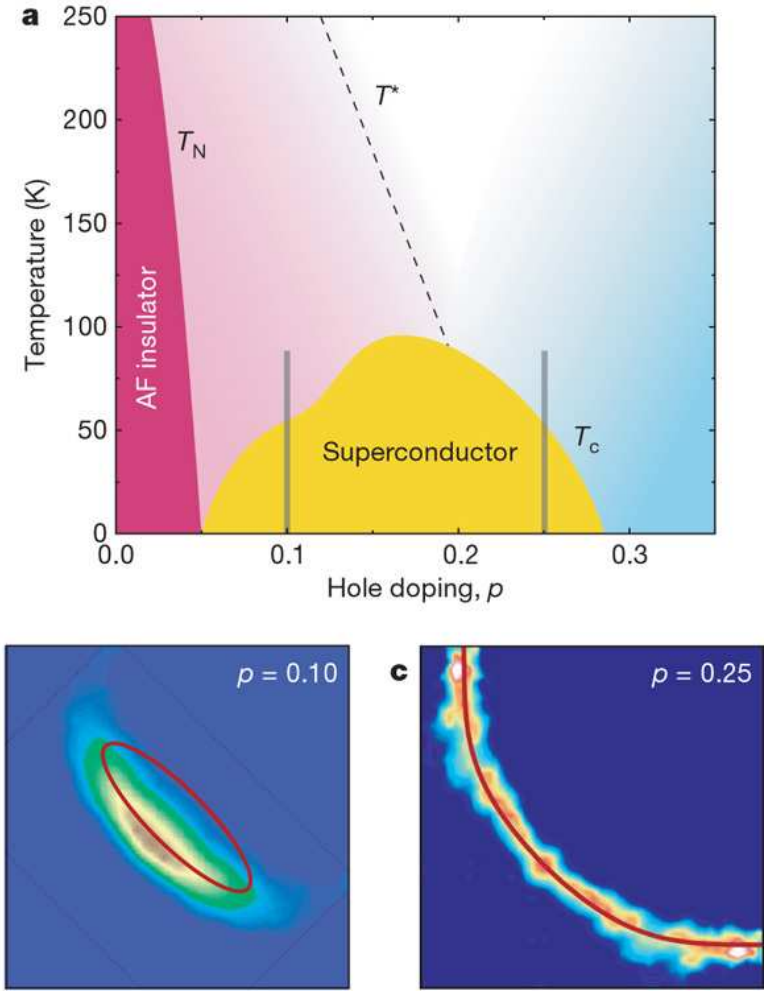




(Data from W. J. Padilla *et al.*, PRB **72**,060511 (2005) - remember: $n_e = 1 - x$)

Does one see anything like this in experiment?





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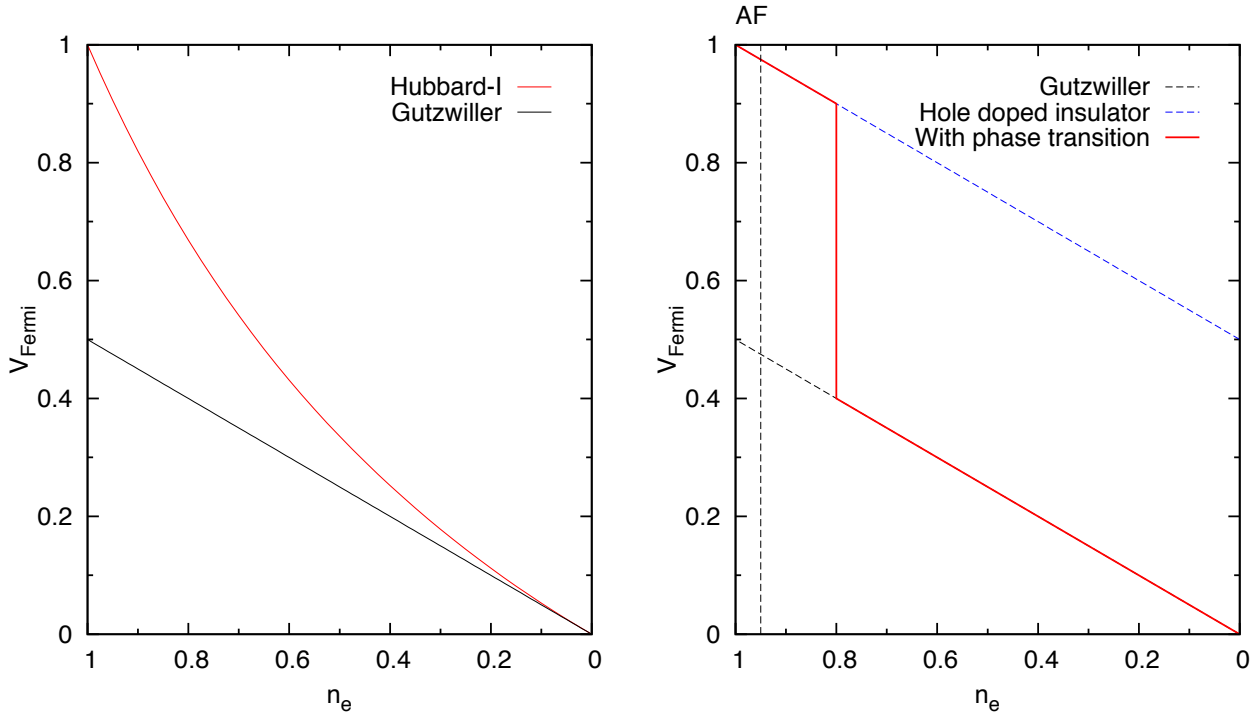

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