Karlsruhe Institute of Technology

The physics of doped Mott insulators

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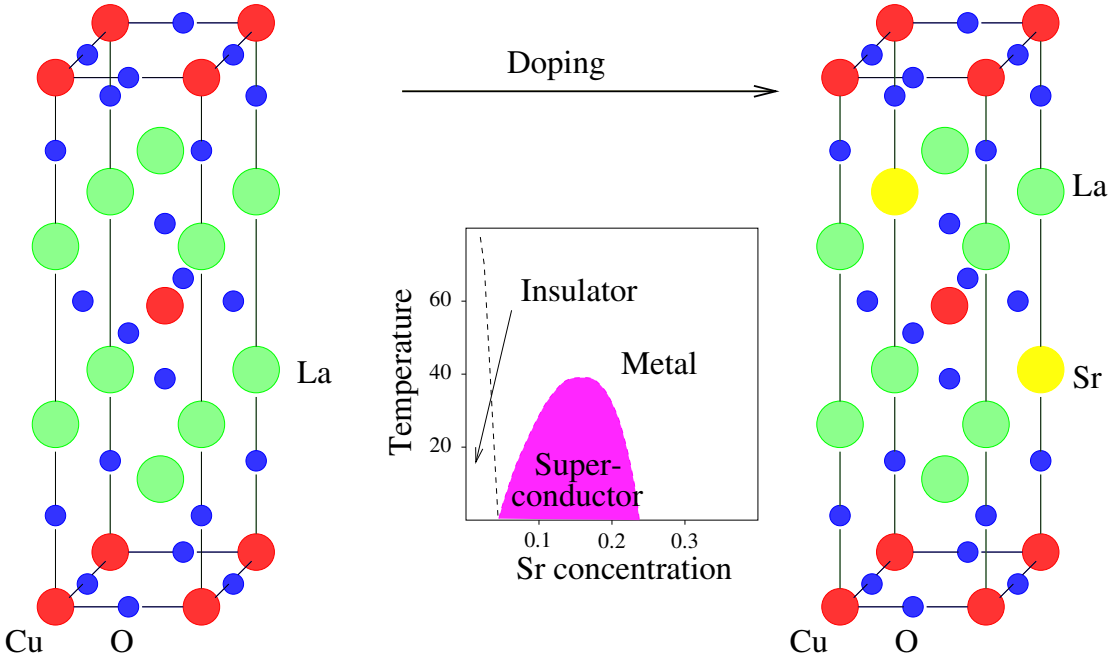
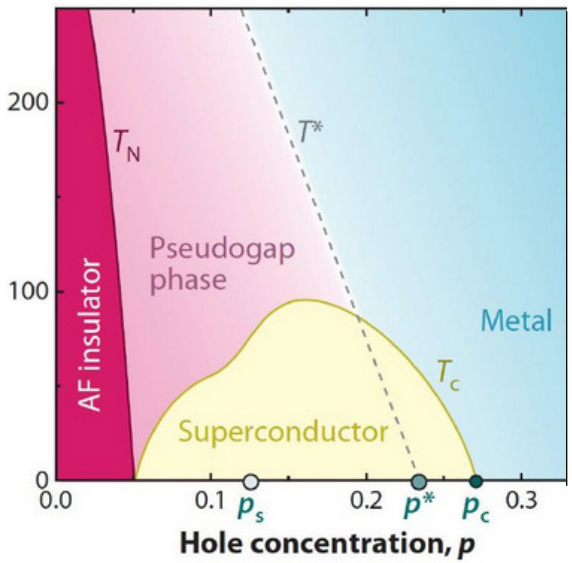
Institute for Quantum Matter and Technologies

Why study doped Mott insulators?

Structure of La_2CuO_4



Phasediagram



Mott insulators

The simplest model to describe Mott insulators is the Hubbard model

$$
\begin{aligned}
H &= \sum_{i,j}\sum_{\sigma} t_{ij}\; c^{\dagger}_{i,\sigma} c_{j,\sigma} + U \sum_{i} n_{i,\uparrow}\, n_{i,\downarrow} \\
&= \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}}\; c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + U \sum_{i} n_{i,\uparrow}\, n_{i,\downarrow} \\
\epsilon_{\mathbf{k}} &= \sum_{j} t_{ij}\; e^{i\mathbf{k}\cdot(\mathbf{R}_j - \mathbf{R}_i)}
\end{aligned}
$$

- We consider this model on a 2D square lattice with N sites
- We denote the number of electrons with spin σ by N_σ and $N_e = N_\uparrow + N_\downarrow$
- Densities are denoted by n, for example $n_e = N_e / N$

Reminder concerning band filling

- The number of **k**-points in the Brillouin zone always is equal to the number of unit cells - in our case N
- One **k**-point can take up two electrons - spin-$\uparrow$ and spin-$\downarrow$
- $N_e = N$ means that the lowest $N/2$ **k**-points contain two electrons each

  - the band is half-filled
- $N_e = 2N$ means that every **k**-point contains two electrons

  - the band is completely filled

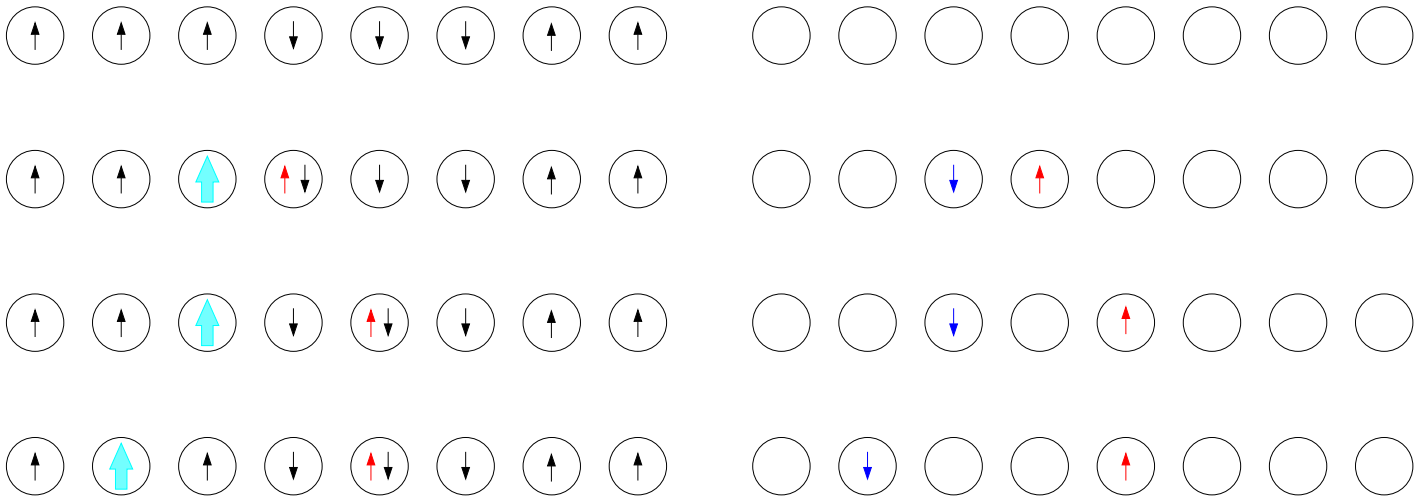
The Hubbard-I approximation

- Consider the Hubbard model at half-filling, $N_\uparrow = N_\downarrow = N/2 \rightarrow N_e = N$
- Set $U/t = \infty \rightarrow$ GS has one electron/site and is highly degenerate

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

- Despite this we assume that there is a unique 'spin background' $|\Psi_0\rangle$
- $|\Psi_0\rangle$ has one electron/site
- Main assumption: $|\Psi_0\rangle$ is 'disordered'
- Now let $U/t < \infty$ but still $t \ll U \rightarrow$ charge fluctuations

Now interpret the charge fluctuations as ‘particles’



- Describe these ‘particles’ by a Hamiltonian

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

Recall ...

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

- Fourier transform:

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

- This quadratic form can be solved by unitary transformation

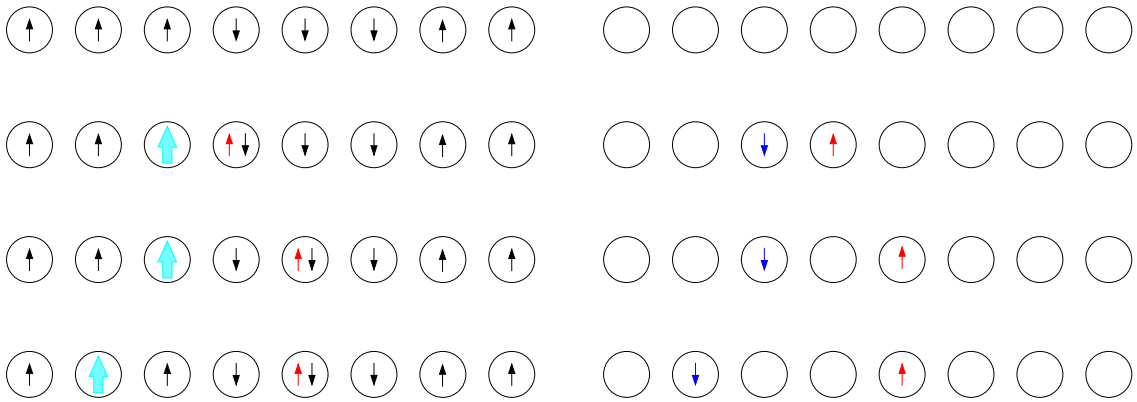
$$\begin{aligned}\gamma^{\dagger}_{\mathbf{k},+,\sigma} &= u_{\mathbf{k}}\, d^{\dagger}_{\mathbf{k},\sigma} + v_{\mathbf{k}}\, h_{-\mathbf{k},-\sigma}\\ \gamma^{\dagger}_{\mathbf{k},-,\sigma} &= -v_{\mathbf{k}}\, d^{\dagger}_{\mathbf{k},\sigma} + u_{\mathbf{k}}\, h_{-\mathbf{k},-\sigma}\end{aligned}$$

Demanding $[H, \gamma^{\dagger}_{\mathbf{k},\alpha,\sigma}] = E_{\mathbf{k},\alpha}\, \gamma^{\dagger}_{\mathbf{k},\alpha,\sigma}$ gives $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ and the two Hubbard bands

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

Electron count

- We need to determine the electron number N_e - recall:



- The vacuum $|\Psi_0\rangle$ has one electron/site $\rightarrow N_e = N$
- A double occupancy $d^\dagger_{i,\sigma}$ increases N_e by 1, a hole $h^\dagger_{i,-\sigma}$ decreases N_e by 1

$$N_e = N + \sum_{i,\sigma} \left(d^\dagger_{i,\sigma} d_{i,\sigma} - h^\dagger_{i,\sigma} h_{i,\sigma} \right)$$

Electron count

- We had

$$
\begin{aligned}
N_e &= \sum_{i,\sigma} \left(d^\dagger_{i,\sigma} d_{i,\sigma} - h^\dagger_{i,\sigma} h_{i,\sigma} \right) + N \\
&= \sum_{\mathbf{k},\sigma} \left(d^\dagger_{\mathbf{k},\sigma} d_{\mathbf{k},\sigma} - h^\dagger_{-\mathbf{k},-\sigma} h_{-\mathbf{k},-\sigma} \right) + N \\
&= \sum_{\mathbf{k},\sigma} \left(d^\dagger_{\mathbf{k},\sigma} d_{\mathbf{k},\sigma} + h_{-\mathbf{k},-\sigma} h^\dagger_{-\mathbf{k},-\sigma} \right) - N \\
&= \sum_{\mathbf{k},\alpha,\sigma} \gamma^\dagger_{\mathbf{k},\alpha,\sigma} \gamma_{\mathbf{k},\alpha,\sigma} - N
\end{aligned}
$$

For $N_e = N$ this means $\left\langle \sum_{\mathbf{k},\alpha,\sigma} \gamma^\dagger_{\mathbf{k},\alpha,\sigma} \gamma_{\mathbf{k},\alpha,\sigma} \right\rangle = 2N$

The lower band is completely filled, the upper completely empty - Mott insulator

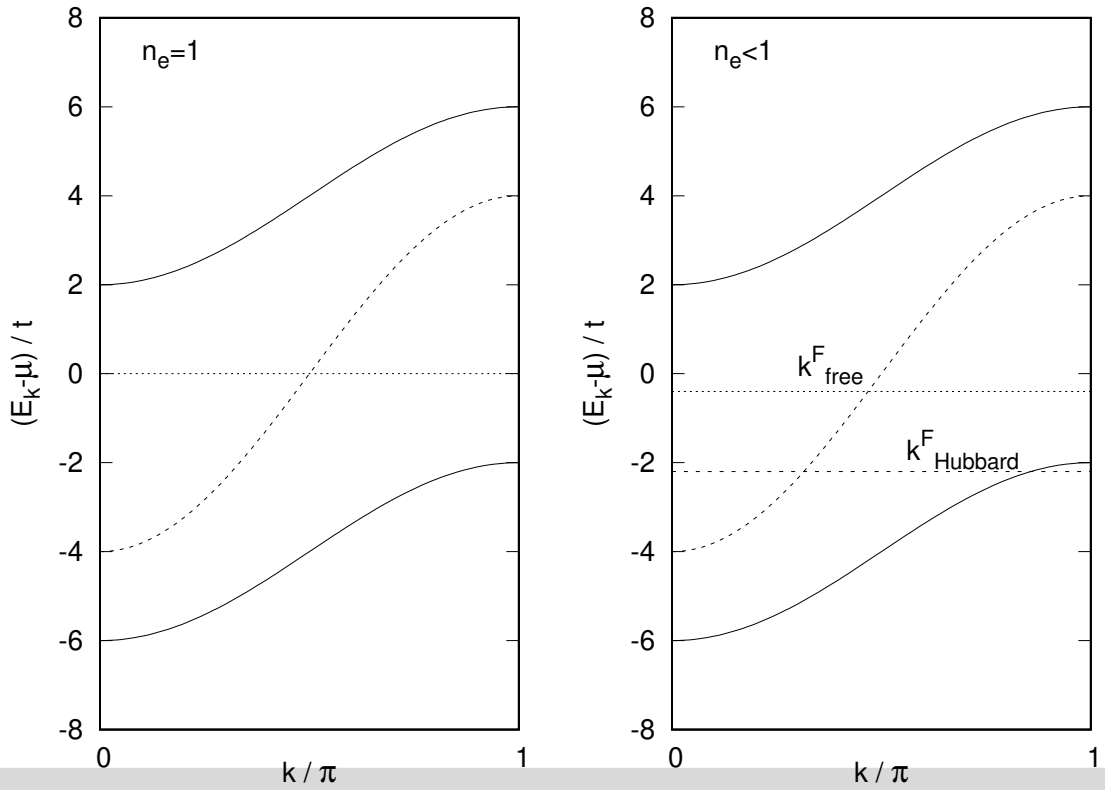
For $N_e = N(1-\delta)$ $\left\langle \sum_{\mathbf{k},\alpha,\sigma} \gamma^\dagger_{\mathbf{k},\alpha,\sigma} \gamma_{\mathbf{k},\alpha,\sigma} \right\rangle = N(2-\delta)$

The lower band has a hole-like Fermi surface with volume $\frac{\delta}{2}\ V_{BZ}$

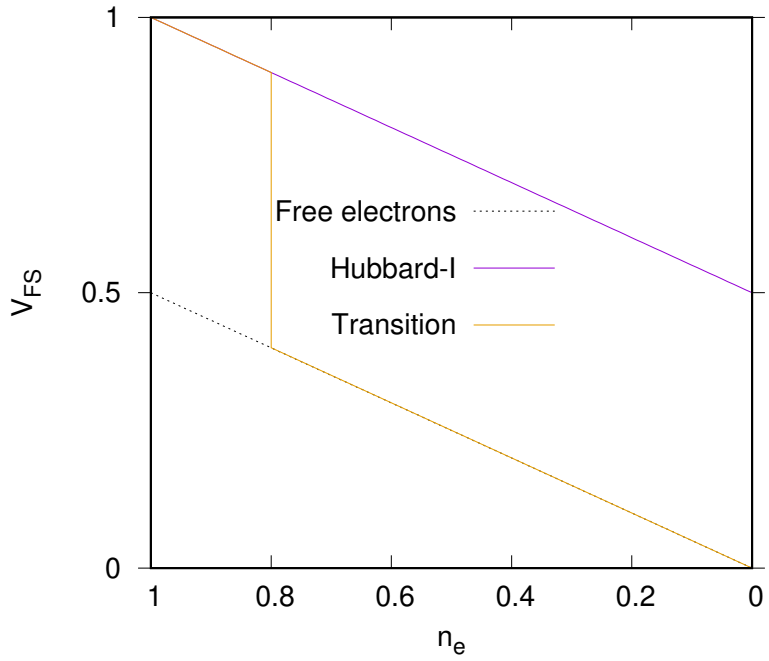
$N_e = N(1-\delta) \rightarrow n_e = 1-\delta$)

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

$$\langle \sum_{\mathbf{k},\alpha,\sigma} \gamma^{\dagger}_{\mathbf{k},\alpha,\sigma}\gamma_{\mathbf{k},\alpha,\sigma} \rangle = 2N(1-\frac{\delta}{2})$$



Fermi surface volume versus doping



- For $n_e \to 0$ we expect free electron behaviour
- This may imply a phase transition
- At $n_e \approx 0.25$ every electron has an empty site next to it $\to$ phase transition

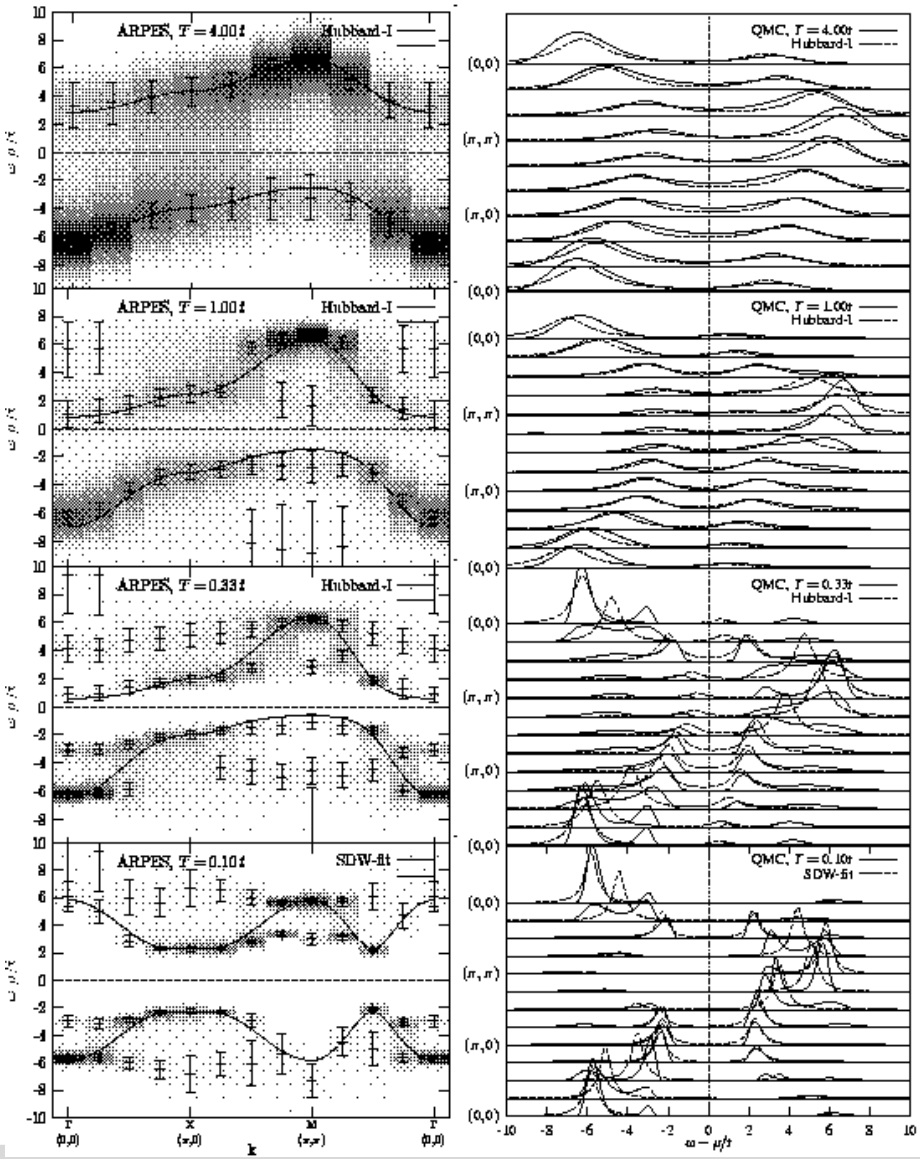
Comparison with Quantum Monte Carlo

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

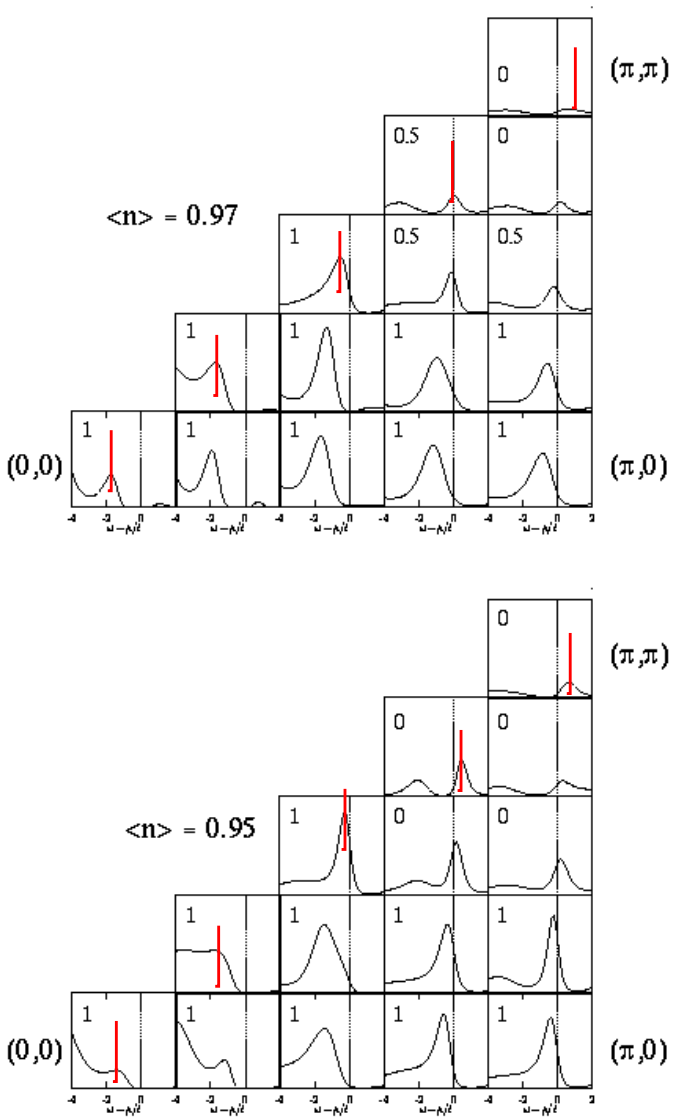
on an 8×8 cluster $U/t = 8$, $n_e = 1$

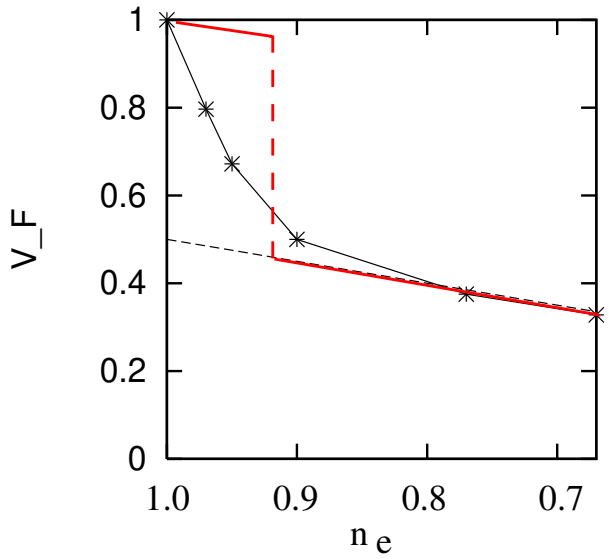
C. Gröber *et al*, PRB **62**, 4336 (2000)

$k_B T = 4t, t, 0.33\ t, 0.1t$ (top to bottom)



Fermi surface volume versus n_e, $k_B T = 4t$





Caveat

- We have represented holes and double occupancies as spinfull particles:

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

But a hole and a double occupancy are spinless objects ?

- $|\Psi_0\rangle$ has definite $S_z \rightarrow c_{i,\uparrow}|\Psi_0\rangle$ and $c_{i,\downarrow}|\Psi_0\rangle$ are orthogonal
- This is despite the hole at i is spinless $\rightarrow$ information about 'spin of missing electron' is 'stored elsewhere'
- The spin-information may 'stay with the hole' or 'go its own way'
- The first scenario would be a Fermi liquid of spin-$\frac{1}{2}$ quasiparticles - the second one is called spin charge separation

We have seen that ...

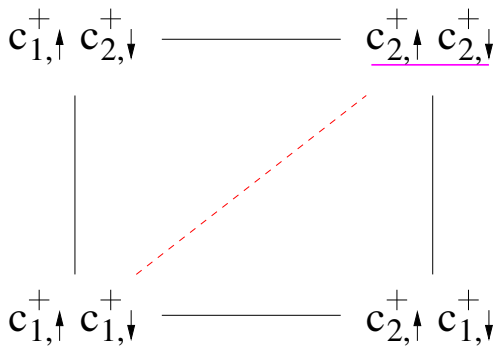
- In a the Hubbard model for large U/t the strong Coulomb repulsion between electrons invalidates the band-description
- Rather, for electron density $n_e = 1$ the ground state may be viewed as a dilute gas of hole-like and double-occupancy-like charge fluctuations populating a 'spin background' with one electron/site
- The electron occupation of each site is close to 1 $\rightarrow$ each site carries a nonvanishing spin
- We have elegantly bypassed this problem by assuming an unspecified 'disordered spin background' $|\Psi_0\rangle$
- Let us now discuss what the spins are really doing

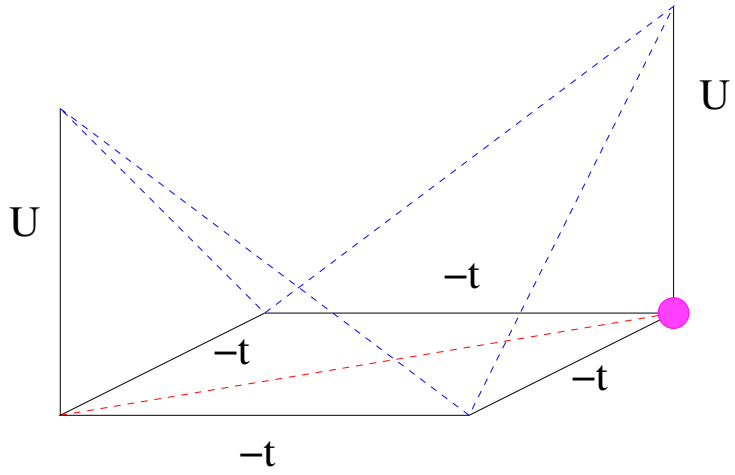
Kinetic spin exchange in Mott insulators

- We consider a Hubbard dimer with $N_\uparrow = N_\downarrow = 1$

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

- This is equivalent to a fictitious particle living on a 2×2 plaquette





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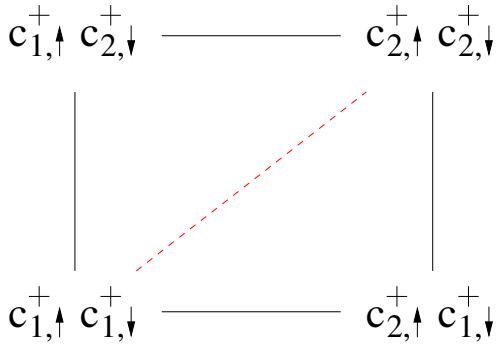
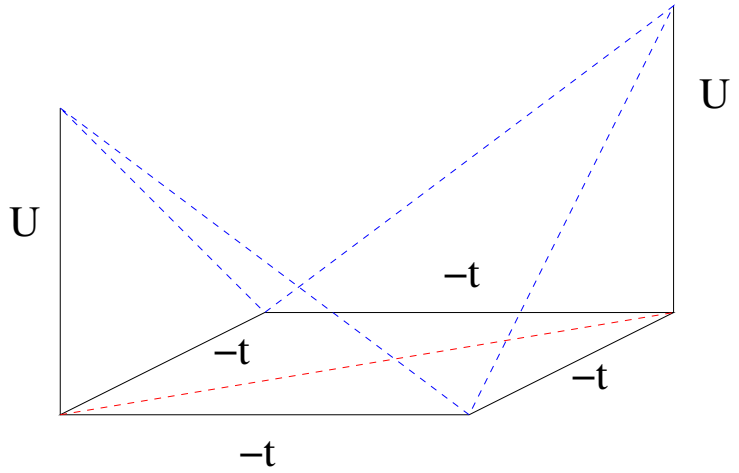




- Eigenstates can be classified by their parity under reflection by the diagonal

$$|\phi_\pm\rangle = \frac{1}{\sqrt{2}}\left(c^\dagger_{1,\uparrow}c^\dagger_{2,\downarrow} \pm c^\dagger_{2,\uparrow}c^\dagger_{1,\downarrow}\right)|0\rangle = \frac{1}{\sqrt{2}}\left(c^\dagger_{1,\uparrow}c^\dagger_{2,\downarrow} \mp c^\dagger_{1,\downarrow}c^\dagger_{2,\uparrow}\right)|0\rangle$$

- $|\phi_+\rangle$ is singlet (S=0), $|\phi_-\rangle$ is triplet (S=1)
- $|\phi_-\rangle$ has zero amplitude on the diagonal $\rightarrow E(S=1) = 0$
- $|\phi_+\rangle$ can 'tunnel' through the barrier $\rightarrow E(S=0) = -C\,\frac{t^2}{U}$
- Detailed calculation shows $C=4 \rightarrow E(S=0) = -\frac{4t^2}{U} = -J$

Kinetic spin exchange in Mott insulators

- We found for two electrons in the dimer:

$$\begin{aligned} E(S=1) &= 0 \\ E(S=0) &= -\frac{4t^2}{U} = -J \end{aligned}$$

- We want to find an 'effective Hamiltonian' which reproduces this level scheme

$$\begin{aligned} S(S+1) = (\mathbf{S}_1 + \mathbf{S}_2)^2 &= \mathbf{S}_1^2 + 2\mathbf{S}_1 \cdot \mathbf{S}_2 + \mathbf{S}_2^2 \\ &= \frac{3}{4} + 2\mathbf{S}_1 \cdot \mathbf{S}_2 + \frac{3}{4} \\ \rightarrow \mathbf{S}_1 \cdot \mathbf{S}_2 &= \frac{1}{2}\left(S(S+1) - \frac{3}{2}\right) = \begin{cases} -\frac{3}{4} & S=0 \\ \frac{1}{4} & S=1 \end{cases} \end{aligned}$$

- Therefore we can summarize the energy levels of the dimer by

$$H_{eff} = J\left(\mathbf{S}_1 \cdot \mathbf{S}_2 - \frac{1}{4}\right)$$

Kinetic spin exchange in Mott insulators

- We generalize this to the lattice by using this H_{eff} for every nearest-neighbor bond - this is the Heisenberg antiferromagnet

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

$J = \frac{4t^2}{U} > 0$ and we have introduced the spin-raising and -lowering operators

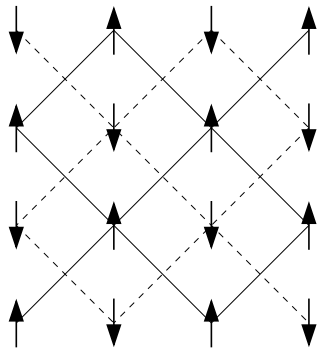
$$
\begin{aligned}
S^+ &= S^x + iS^y \\
S^- &= S^x - iS^y
\end{aligned}
\quad \Rightarrow \quad
\begin{aligned}
S^x &= \tfrac{1}{2}(S^+ + S^-) \\
S^y &= \tfrac{1}{2}(S^- - S^+)
\end{aligned}
$$

The 2d Heisenberg antiferromagnet

- We consider a 2d square lattice with exchange only between nearest neighbors

$$H = J \sum_{\langle i,j \rangle} \left(\frac{1}{2} \left(S_i^+ S_j^- + S_i^- S_j^+ \right) + S_i^z S_j^z \right)$$

- If only the term $\propto J\, S_i^z\, S_j^z$ were present the ground state is the Néel state



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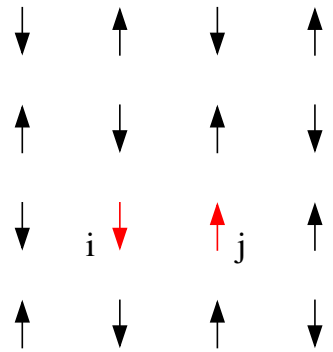
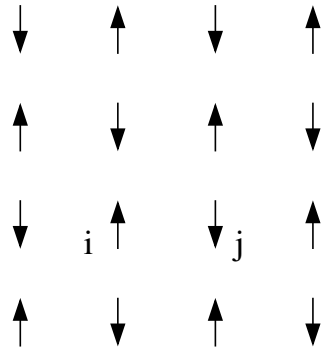


- The Néel state is not an eigenstate of the full Hamiltonian because the term $\propto S_i^+ S_j^- + S_i^- S_j^+$ produces quantum fluctuations

Linear spin wave theory

More on quantum fluctuations:



Linear spin wave theory

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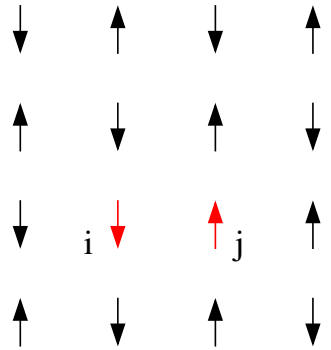

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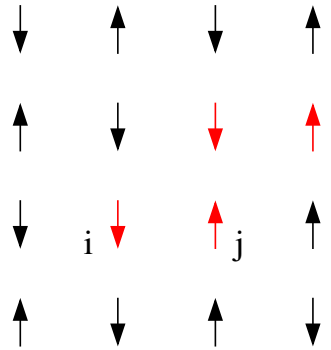

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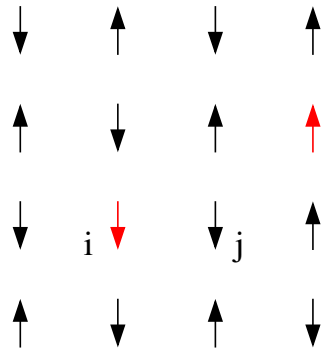

Linear spin wave theory

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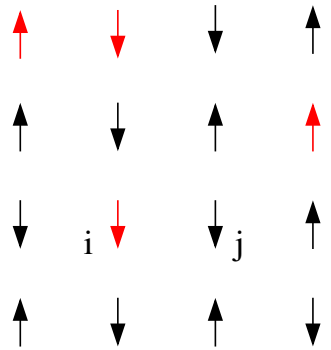
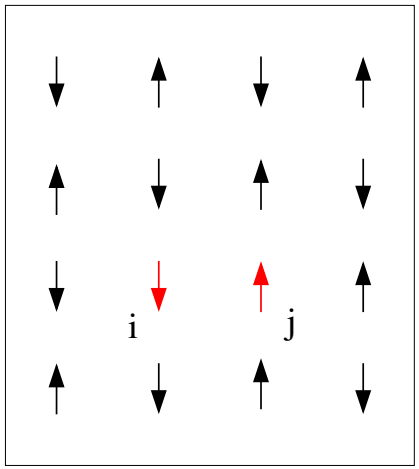
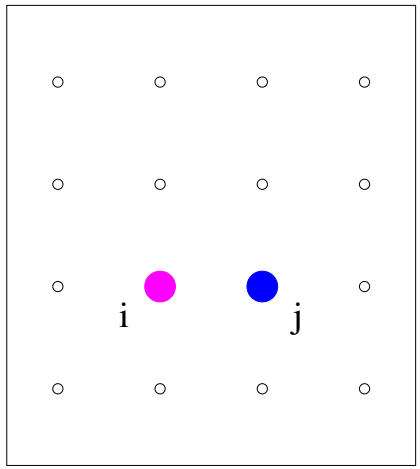


- There are two possible outcomes
- The quantum fluctuations could completely destroy the antiferromagnetic order and a qualitatively new state may ensue
- Or an equilibrium concentrations of inverted spins may be reached and we have an antiferromagnet hosting a gas of magnons
- In one dimension the ground state is disordered in two dimensions or higher the antiferromagnetic order survives $\rightarrow$ we 'expand around the Néel state'

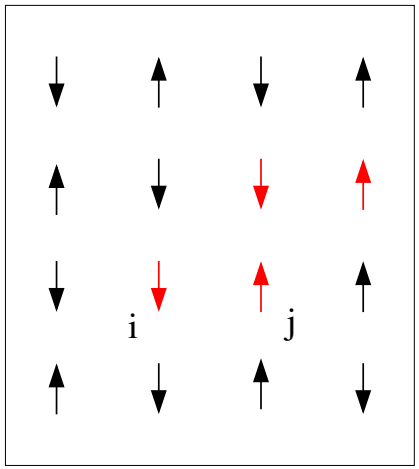
Linear spin wave theory

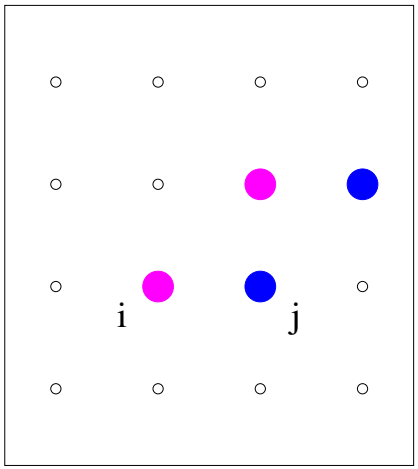




- Consider the Néel state as vacuum $|0\rangle$
- Represent a $\downarrow$-spin at site i on the $\uparrow$-sublattice as a Boson created by $a_i^\dagger$
- Represent a $\uparrow$-spin at site j on the $\downarrow$-sublattice as a Boson created by $b_j^\dagger$

Linear spin wave theory





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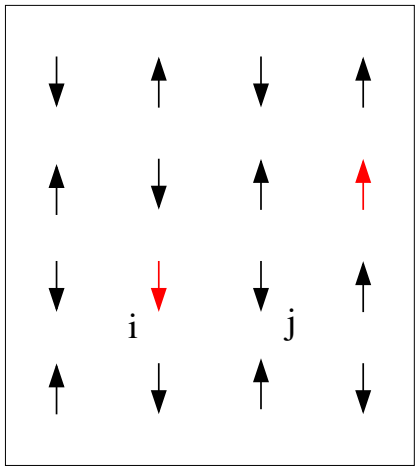
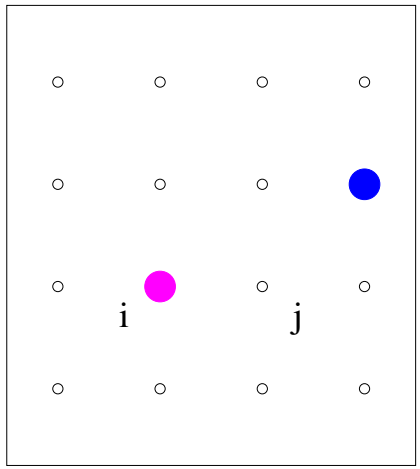
Linear spin wave theory





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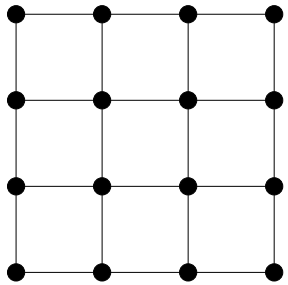
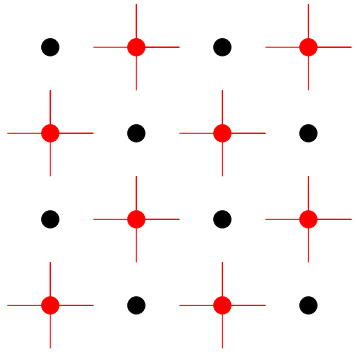
- Represent a $\uparrow$-spin at site j on the $\downarrow$-sublattice as a Boson created by $b_j^\dagger$
- Why Bosons? - Spin operators on different sites commute!
- States like $(a_i^\dagger)^2|0\rangle$ are meaningless
- Additional constraint: at most one Boson/site - 'hard core constraint'

Hamiltonian for spin fluctuations

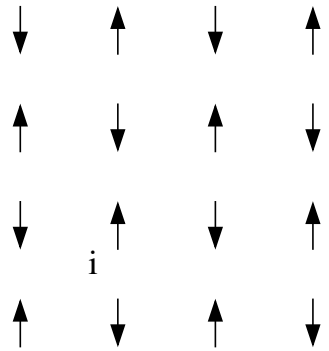
- Represent a $\downarrow$-spin at site i on the $\uparrow$-sublattice as a Boson created by $a_i^\dagger$
- Represent a $\uparrow$-spin at site j on the $\downarrow$-sublattice as a Boson created by $b_j^\dagger$

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





Hamiltonian for spin fluctuations



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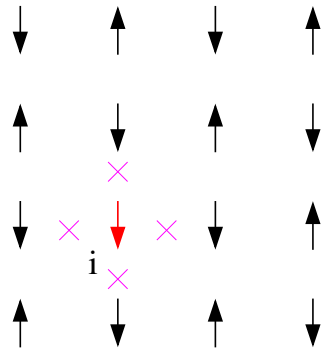


- If one spin is inverted $z = 4$ bonds switch from $(\uparrow, \downarrow)$ to $(\downarrow, \downarrow)$
- $J\ S_i^z\ S_j^z$ changes from $-\frac{J}{4}$ to $\frac{J}{4}$ for these bonds
- The total increase in energy is $\frac{zJ}{2}$
- We interpret this as the energy of the boson

$$J \sum_{\langle i,j \rangle} S_i^z\ S_j^z \quad = \quad E_{Neel} + \frac{zJ}{2} \left(\sum_{i \in A} a_i^\dagger a_i + \sum_{j \in B} b_j^\dagger b_j \right)$$

Hamiltonian for spin fluctuations

Collecting everything we find the spin wave Hamiltonian

$$H_{SW} = \frac{zJ}{2}\left(\sum_{i\in A} a_i^\dagger\, a_i + \sum_{i\in B} b_i^\dagger\, b_i\right) + \frac{J}{2}\sum_{i\in A}\sum_{\mathbf{n}}\left(a_i^\dagger\, b_{i+\mathbf{n}}^\dagger + b_{i+\mathbf{n}}\, a_i\right).$$

We switch to Fourier transformed operators ...

$$a_{\mathbf{k}}^\dagger = \sqrt{\frac{2}{N}}\sum_{j\in A} e^{i\mathbf{k}\cdot\mathbf{R_j}}\, a_j^\dagger \qquad b_{\mathbf{k}}^\dagger = \sqrt{\frac{2}{N}}\sum_{j\in B} e^{i\mathbf{k}\cdot\mathbf{R_j}}\, b_j^\dagger$$

... and find

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

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

Solving the Hamiltonian

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

- H_{SW} can be diagonalized by a Bosonic Bogoliubov transformation
- We define new Bosonic operators $\alpha_{\mathbf{k}}^\dagger$ and $\beta_{\mathbf{k}}^\dagger$ by ...

$$\begin{aligned} \alpha_{\mathbf{k}}^\dagger &= u_{\mathbf{k}} \; a_{\mathbf{k}}^\dagger + v_{\mathbf{k}} \; b_{-\mathbf{k}} \\ \beta_{-\mathbf{k}}^\dagger &= u_{\mathbf{k}} \; b_{-\mathbf{k}}^\dagger + v_{\mathbf{k}} \; a_{\mathbf{k}} \end{aligned}$$

... and demand that they obey Bosonic commutation rules and diagonalize H_{SW}

$$\left[\alpha_{\mathbf{k}}, \alpha_{\mathbf{k}'}^\dagger \right] = \left[\beta_{\mathbf{k}}, \beta_{\mathbf{k}'}^\dagger \right] = \delta_{\mathbf{k},\mathbf{k}'} \qquad \left[H_{SW}, \alpha_{\mathbf{k}}^\dagger \right] = \omega_{\mathbf{k}} \; \alpha_{\mathbf{k}}^\dagger$$

- This gives (see notes) $u_{\mathbf{k}}$, $v_{\mathbf{k}}$ and $\omega_{\mathbf{k}} = \frac{zJ}{2} \sqrt{1 - \gamma_{\mathbf{k}}^2}$

Spin waves

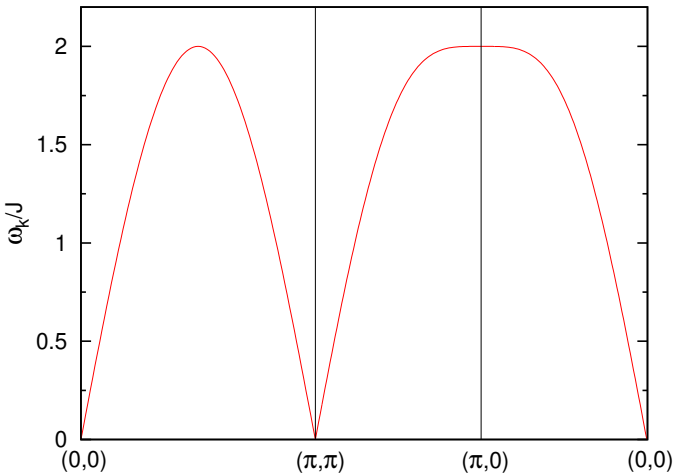
- Recall

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

- Band width: $2J$

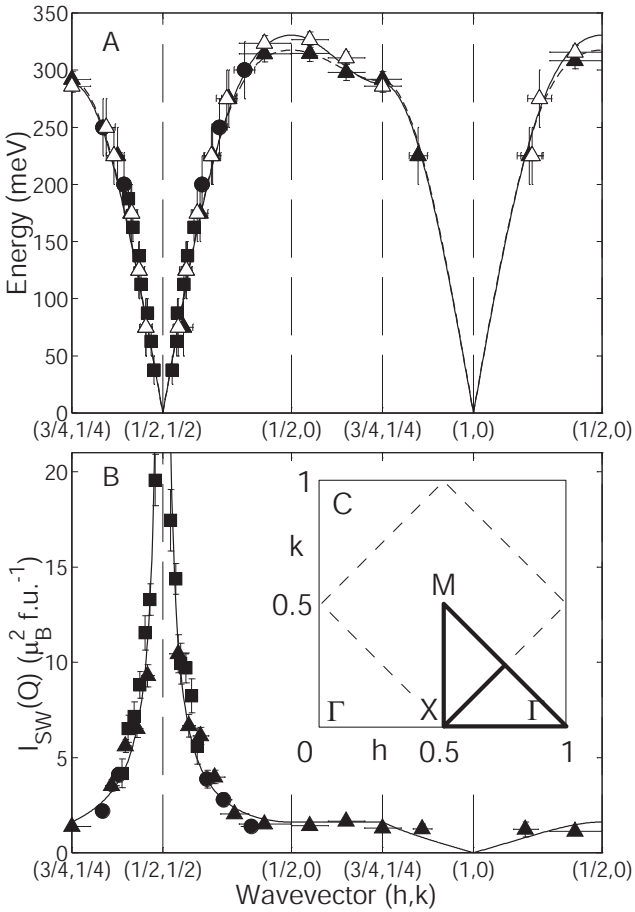
$$\gamma_{\mathbf{k}} = \frac{1}{4}\left(2\cos(k_x)+2\cos(k_y)\right) \overset{k\to 0}{\longrightarrow} 1-\frac{1}{4}\left(k_x^2+k_y^2\right)+\ldots$$

$$\omega_{\mathbf{k}} \overset{k\to 0}{\longrightarrow} J\sqrt{2}\,|\mathbf{k}|$$



Spin waves in experiment

Result of inelastic neutron scattering experiments on La_2CuO_4



Bandwidth $\approx$ 300meV$\Rightarrow$ $J \approx$ 150meV

Good fit with additional ring exchange

$J \Rightarrow =$ 138meV

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

We have seen that ...

- In a Mott-insulator electrons are localized $\rightarrow$ spin-$\frac{1}{2}$ at each site
- The spins 'communicate' by hopping $\rightarrow$ Heisenberg Hamiltonian
- In $d \geq 2$ this results in antiferromagnetic order
- Spins which are inverted relative to the order aquire the nature of propagating Bosonic excitations: spin waves
- Doped holes have to move through this 'spin environment'
- This will modify their motion - which is what we will discuss next

Doped Mott insulators

- To describe the doped Mott insulator we have to upgrade the Heisenberg antiferromagnet and add some mobile vacancies
- This is described by the famous t-J model

$$H_{t-J} = -t \sum_{\langle i,j \rangle} \sum_{\sigma} \left(\hat{c}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} + H.c. \right) + J \sum_{\langle i,j \rangle} \left(\frac{1}{2} \left(S^{+}_{i} S^{-}_{j} + S^{-}_{i} S^{+}_{j} \right) + S^{z}_{i} S^{z}_{j} \right)$$

The Hubbard operator $\hat{c}^{\dagger}_{i,\sigma} = c^{\dagger}_{i,\sigma}(1 - n_{i,\bar{\sigma}})$ creates an electron only on empty sites

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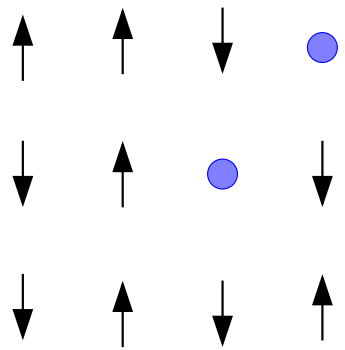

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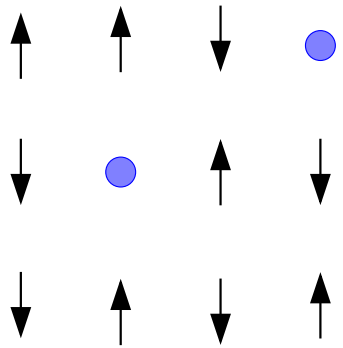

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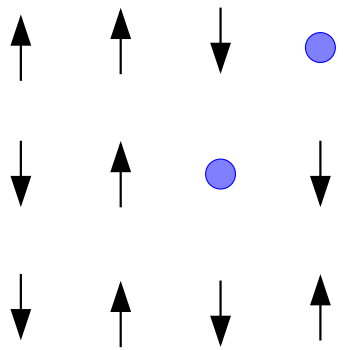

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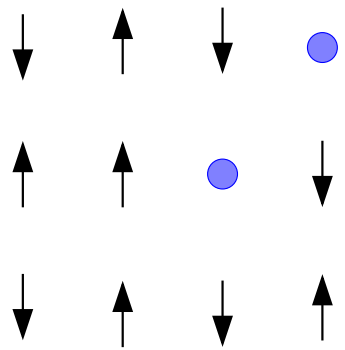

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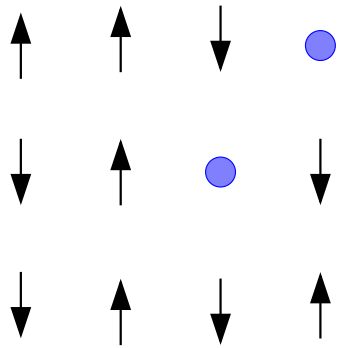

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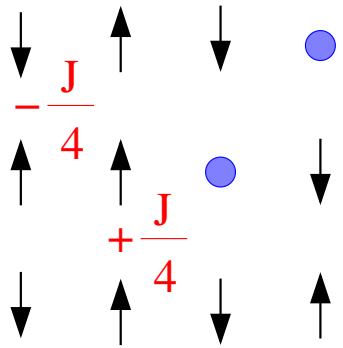


Doped Mott insulators

The t-J model

$$H_{t-J} = -t \sum_{\langle i,j \rangle} \sum_{\sigma} \left(\hat{c}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} + H.c. \right) + J \sum_{\langle i,j \rangle} \left(\frac{1}{2} \left(S_i^+ S_j^- + S_i^- S_j^+ \right) + S_i^z S_j^z \right)$$

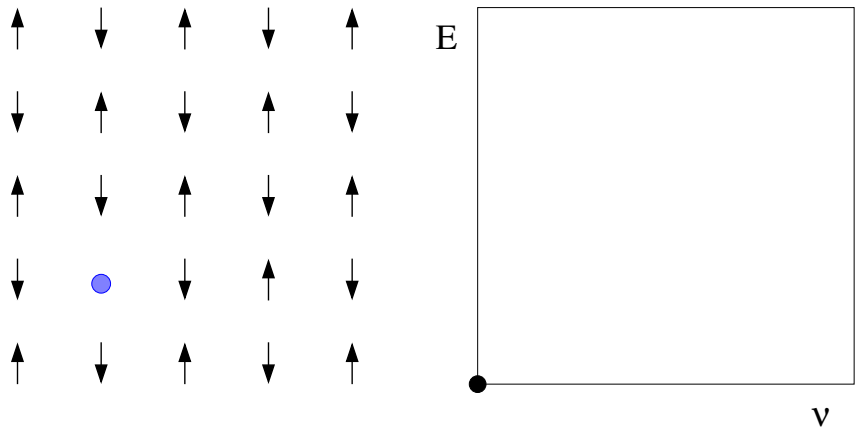
- It was derived by Chao, Spałek and Oleś as the strong coupling limit of the Hubbard model, J. Phys. C10, L **271** (1977)
- It was shown to describe the CuO_2-planes in copper oxide superconductors by Zhang and Rice, Phys. Rev. B **37**, 3759 (1988)
- Parameter values to describe the CuO_2 planes of copper oxide superconductors are $t \approx 350\text{meV}$ and $J \approx 140\text{meV}$, so $J/t = 0.4$

Hole in an antiferromagnet

- We consider the case $N_e = N - 1$ - a single hole in an antiferromagnet

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

- A single hole will not affect the magnetic order $\Rightarrow$ we start from the Néel state



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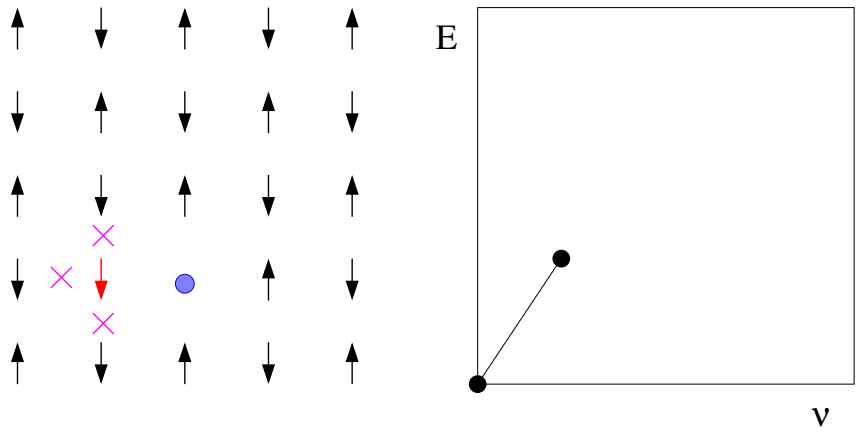

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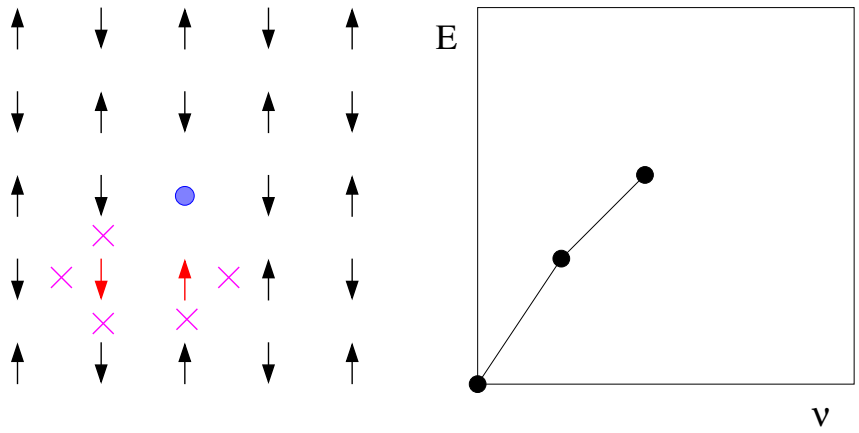

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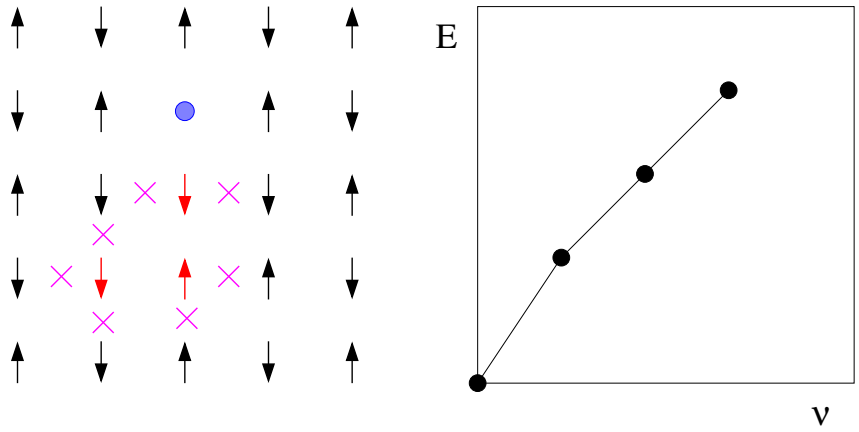

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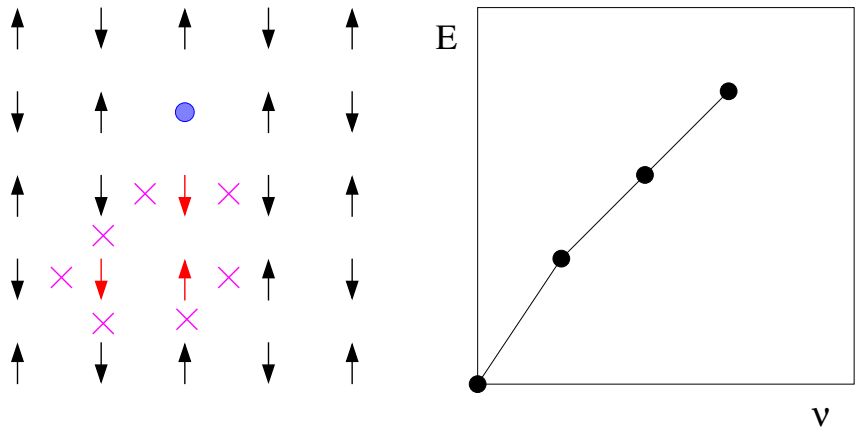
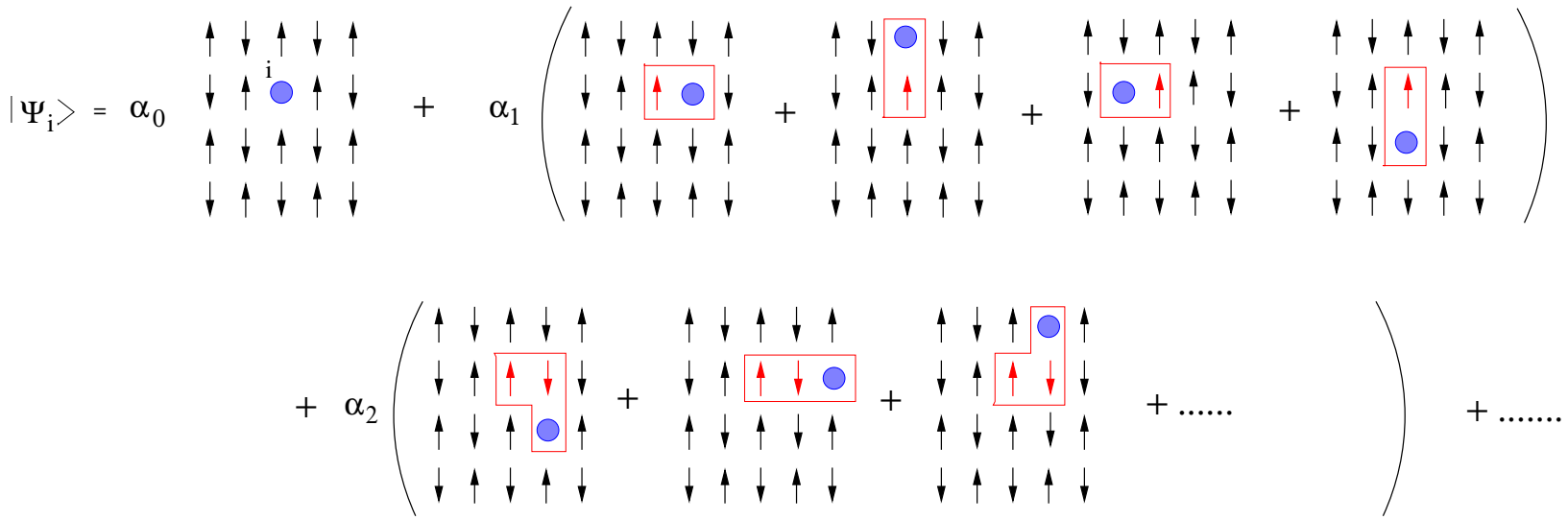


- The magnetic energy increases linearly with the number of steps
- The hole is self-trapped

- Variational wave function for the self-trapped state at site *i*



- We decompose the t-J Hamiltonian ...

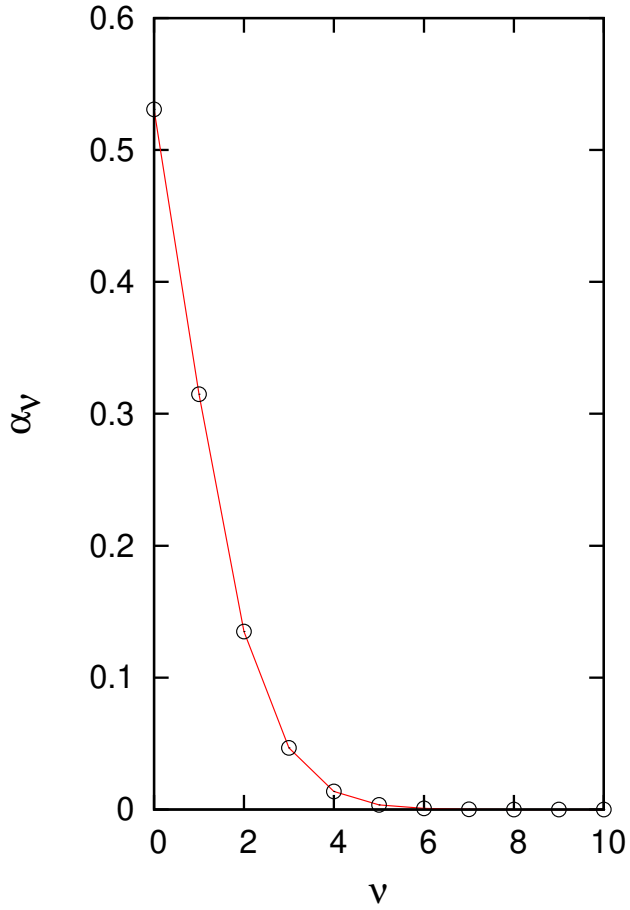
$$H_t = -t \sum_{\langle i,j \rangle} \sum_{\sigma} (\hat{c}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} + H.c) \qquad H_I = J \sum_{\langle i,j \rangle} S^z_i S^z_j \qquad H_{\perp} = \frac{J}{2} \sum_{\langle i,j \rangle} \left(S^+_i S^-_j + S^-_i S^+_j \right)$$

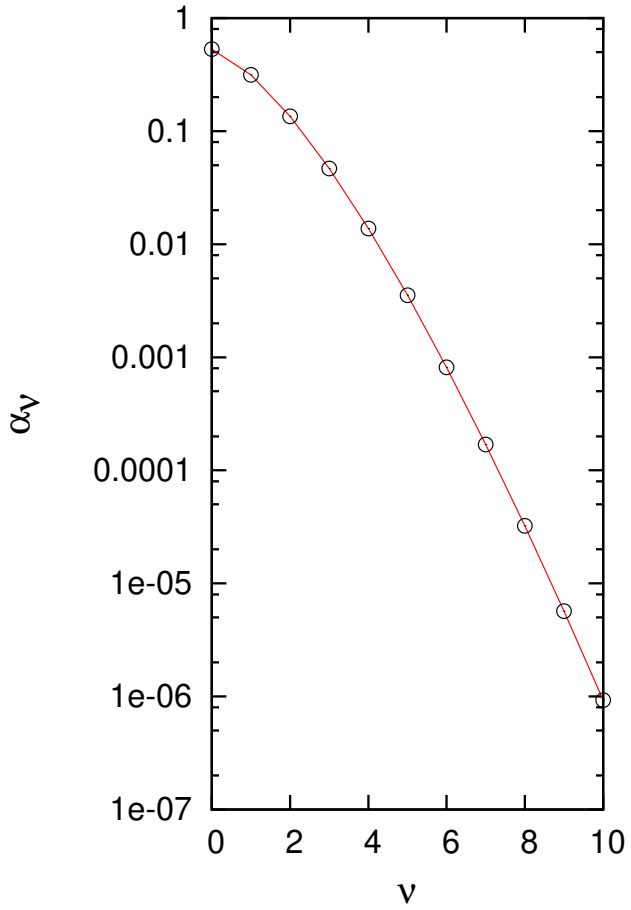
... and determine the coefficients α_ν variationally (see notes)

$$E_{loc} = \frac{\langle \Psi_i | H_t + H_I | \Psi_i \rangle}{\langle \Psi_i | \Psi_i \rangle} \rightarrow min$$

Variational wave function for the self-trapped state at site i

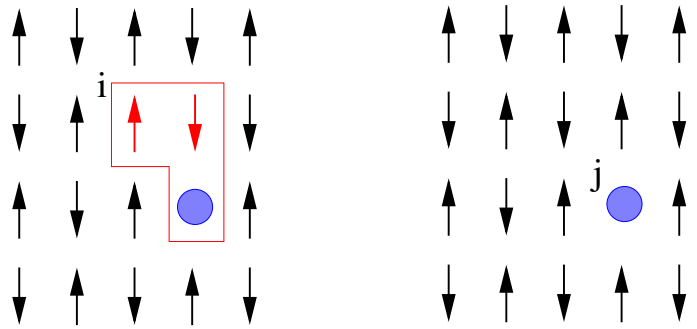
This is what the solution looks like for $J/t = 0.4$





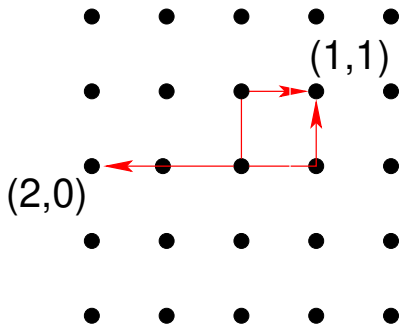
Escape from the trap!

- Increase of magnetic energy leads to formation of self-trapped states $|\Psi_i\rangle$
- However, delocalization due to spin-flip term $H_\perp = \frac{J}{2} \sum_{\langle i,j \rangle} \left(S_i^+ S_j^- + S_i^- S_j^+ \right)$



Matrix element: $\frac{J}{2}\, \alpha_2\, \alpha_0$

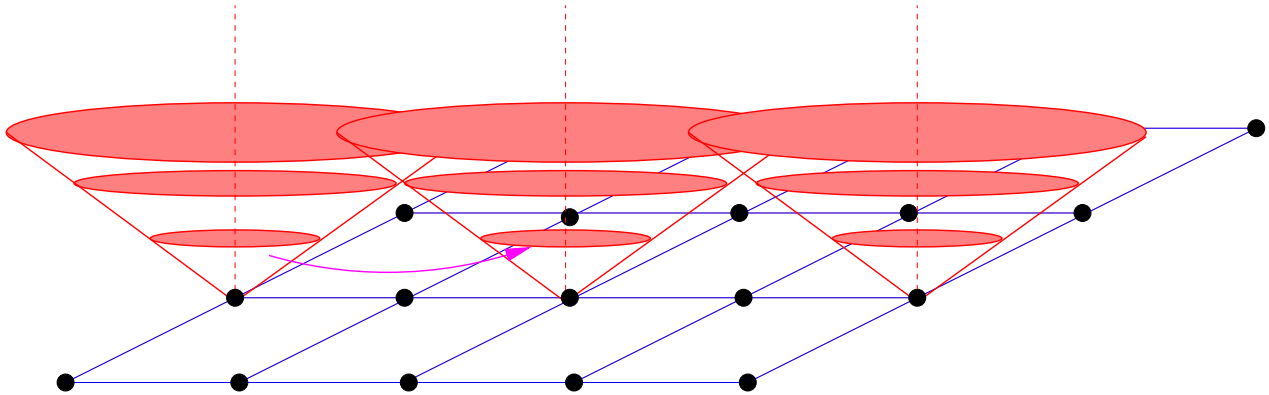
- By 'two steps + 1 spin-flip' the center i of $|\Psi_i\rangle$ is shifted by two lattice sites



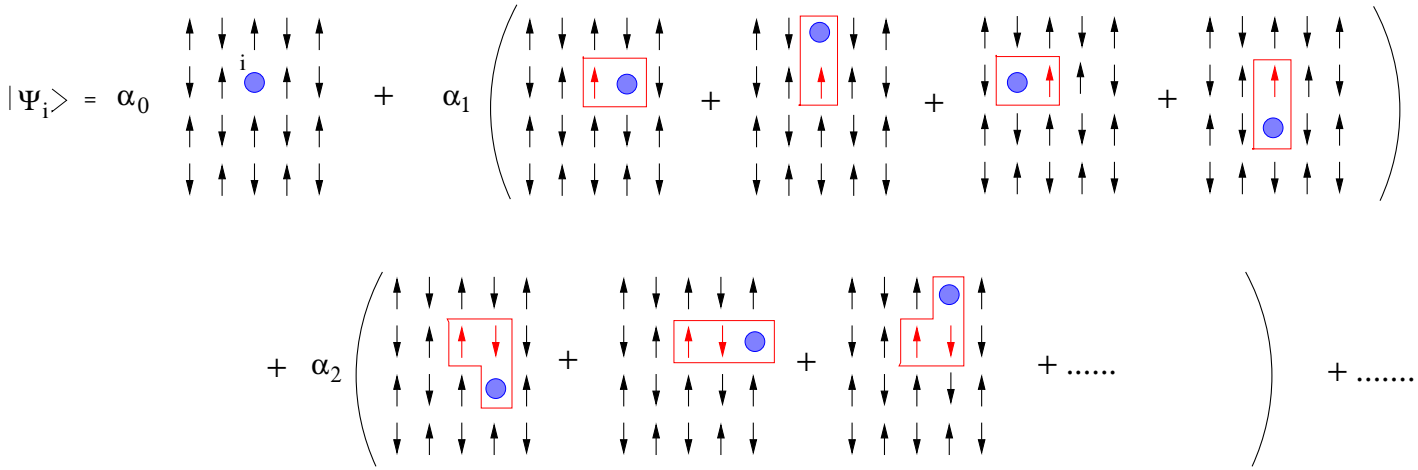
- Hopping to $(1,1)$ and $(2,0)$ like neighbors
- Matrix element to $(1,1) \approx$ twice to $(2,0)$
- Matrix elements $\propto J$ rather than t!

Propagation of the hole

- We arrive at a tight-binding-like picture



Hopping via exchange!



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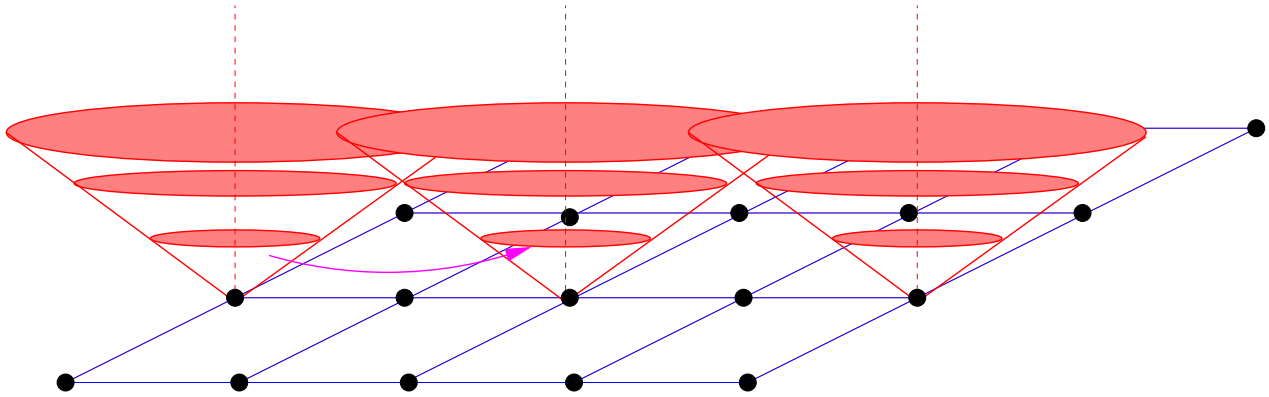


Hopping via exchange!

- A Bloch state of the hole is

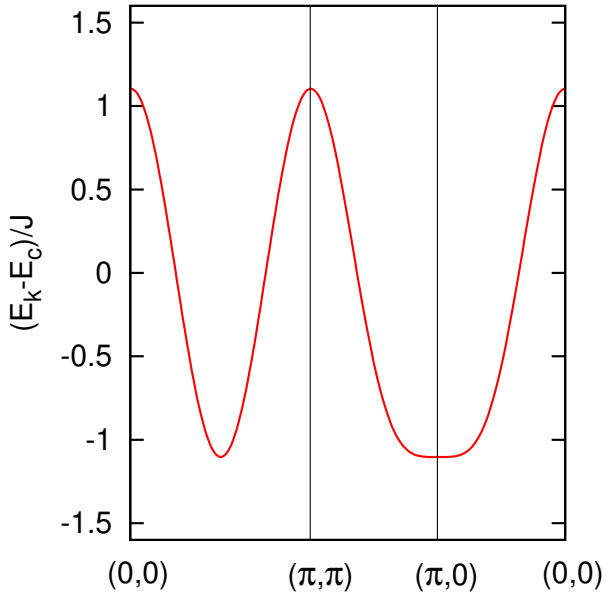
$$|\Psi_{\mathbf{k},\uparrow}\rangle \quad = \quad \sqrt{\frac{2}{N}} \sum_{j \in \uparrow - SL} e^{i\mathbf{k}\cdot\mathbf{R}_j} \, |\Psi_i\rangle$$

- Hopping matrix element due to spin-flip term (see notes)

$$\langle \Psi_j | H_\perp | \Psi_i \rangle \quad = \quad J \sum_{\nu=0}^{\infty} (z-1)^\nu \, \alpha_\nu \alpha_{\nu+2} = J \cdot m$$

Band structure of the hole

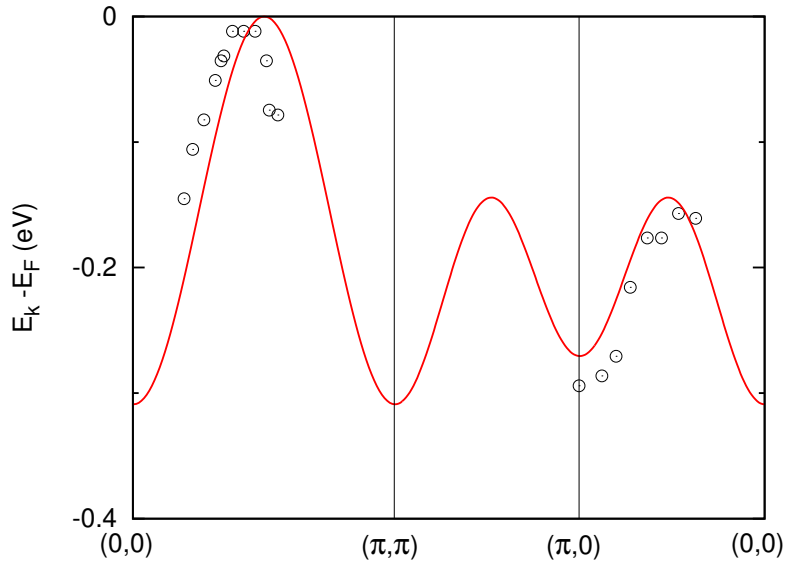
$$E_{\mathbf{k}} = E_{loc} - 4Jm + 4Jm\left[\cos(k_x) + \cos(k_y)\right]^2$$



Note: the bandwidth is $W \approx 2J$ - the free bandwidth would be $W_{free} = 8t$ so that $\frac{W_{free}}{W} = \frac{4t}{J} = 10$ for $J/t = 0.4$ - Massive downward renormalization!

Comparison to experiment

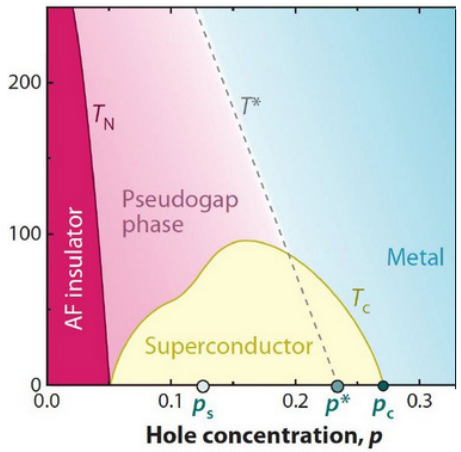
- In actual cuprate materials there are also substantial hopping integrals t' and t'' between $(1,1)$-like and $(2,0)$ like neighbors - these can be included into the present theory (see notes) and we can compare to experiment:



- Band dispersion from ARPES for the AF insulator $Sr_2CuO_2Cl_2$ from S. LaRosa *et al.* PRB **56**, R525(R) (1997)
- Parameter values are $t = 350$meV, $J = 140$meV, $t' = -120$meV, $t'' = 60$meV

We have seen that ...

- The Heisenberg exchange gives the spins a ‘life of their own’ - resulting in antiferromagnetism in the Mott insulator and spin excitations
- The holes move in this ‘spin background’ and - their motion is modified strongly
- For a finite concentration of holes this also goes the other way round - the spins are ‘stirred’ by the holes
- In cuprate superconductors the antiferromagnetic order disappears for hole concentrations of a few percent - our calculations so far become invalid ...



A tough problem

- Whereas it is very easy to write down ordered states it is very difficult to write down a wave function for spins that is
- a) disordered
- b) has one electrons/site
- c) can be treated in any other way than numerically
- Example: a state obtained by simply summing over all 2^N possible spin states should be 'disordered'?

$$|\psi\rangle \quad = \quad \sum_{\sigma_1=\downarrow}^{\uparrow} \sum_{\sigma_2=\downarrow}^{\uparrow} \cdots \sum_{\sigma_N=\downarrow}^{\uparrow} |\sigma_1, \sigma_2, \ldots, \sigma_N\rangle$$

- In reality this is the ferromagnetic state in x-direction: $\prod_i \left(|i,\uparrow\rangle + |i,\downarrow\rangle\right)$

Recap: Dimer basis

The Heisenberg antiferromagnet on a dimer with sites labeled 1 and 2

$$H = J\,\mathbf{S}_1 \cdot \mathbf{S}_2$$

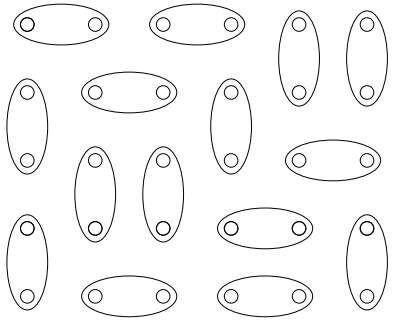
- Eigenstates are the singlet with energy $-\frac{3J}{4}$ and the 3 triplets with energy $\frac{J}{4}$

$$\begin{aligned}
|s\rangle &= \frac{1}{\sqrt{2}}\left(c^\dagger_{1,\uparrow}c^\dagger_{2,\downarrow} - c^\dagger_{1,\downarrow}c^\dagger_{2,\uparrow} \right)|0\rangle \\
|t_x\rangle &= \frac{1}{\sqrt{2}}\left(c^\dagger_{1,\downarrow}c^\dagger_{2,\downarrow} - c^\dagger_{1,\uparrow}c^\dagger_{2,\uparrow} \right)|0\rangle \\
|t_y\rangle &= \frac{i}{\sqrt{2}}\left(c^\dagger_{1,\uparrow}c^\dagger_{2,\uparrow} + c^\dagger_{1,\downarrow}c^\dagger_{2,\downarrow} \right)|0\rangle \\
|t_z\rangle &= \frac{1}{\sqrt{2}}\left(c^\dagger_{1,\uparrow}c^\dagger_{2,\downarrow} + c^\dagger_{1,\downarrow}c^\dagger_{2,\uparrow} \right)|0\rangle
\end{aligned}$$

- The triplets obey $S_\alpha|t_\beta\rangle = i\epsilon_{\alpha\beta\gamma}\,|t_\gamma\rangle \rightarrow$ they form a vector under spin rotations

The singlet soup

- Let the N sites of the plane be partitioned into $N/2$ dimers - each made of two nearest neighbors:



- Let each dimer be covered by a singlet - the resulting state is

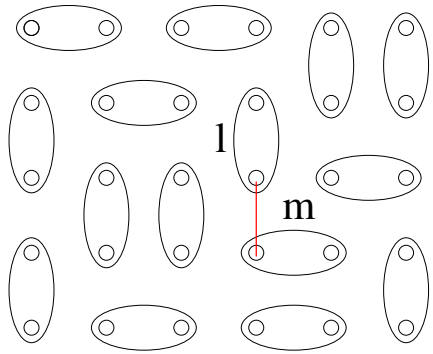
$$|\Psi_0\rangle \quad = \quad \prod_{(i,j)\in D} \frac{1}{\sqrt{2}} \left(c^\dagger_{i,\uparrow} c^\dagger_{j,\downarrow} - c^\dagger_{i,\downarrow} c^\dagger_{j,\uparrow} \right) |0\rangle$$

- D is the set of $N/2$ pairs (i,j) of nearest neighbor sites corresponding to the given dimer covering

- $|\Psi_0\rangle$ is the ground state of the 'depeleted Hamiltonian' $H_d = J \sum_{(i,j)\in D} \mathbf{S}_i \cdot \mathbf{S}_j$

Excitations of the singlet soup

$$|\Psi_0\rangle \quad = \quad \prod_{(i,j)\in D} \frac{1}{\sqrt{2}} \left(c^\dagger_{i,\uparrow} c^\dagger_{j,\downarrow} - c^\dagger_{i,\downarrow} c^\dagger_{j,\uparrow} \right) |0\rangle$$



Let us assume we act with - say - $J\ S^x_i\ S^x_j$ along a bond not included in D

$$S_{1,x}|s\rangle \quad = \quad \frac{1}{2}\left(S^-_1 + S^+_1\right) \frac{1}{\sqrt{2}} \left(c^\dagger_{1,\uparrow} c^\dagger_{2,\downarrow} - c^\dagger_{1,\downarrow} c^\dagger_{2,\uparrow} \right) |0\rangle$$

$$= \quad \frac{1}{2\sqrt{2}} \left(c^\dagger_{1,\downarrow} c^\dagger_{2,\downarrow} - c^\dagger_{1,\uparrow} c^\dagger_{2,\uparrow} \right) |0\rangle = \frac{1}{2}\,|t_x\rangle$$

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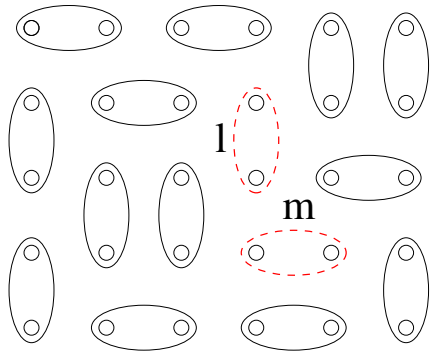

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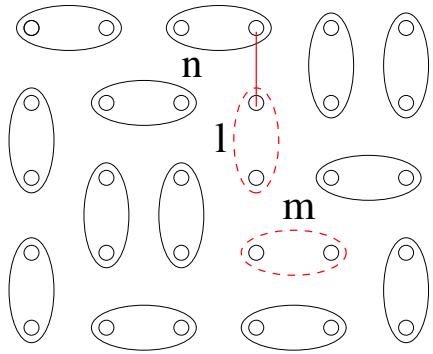

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$$= \frac{1}{2\sqrt{2}} \left(c^\dagger_{1,\uparrow} c^\dagger_{2,\downarrow} - c^\dagger_{1,\downarrow} c^\dagger_{2,\uparrow} \right) |0\rangle = \frac{1}{2}\,|s\rangle$$

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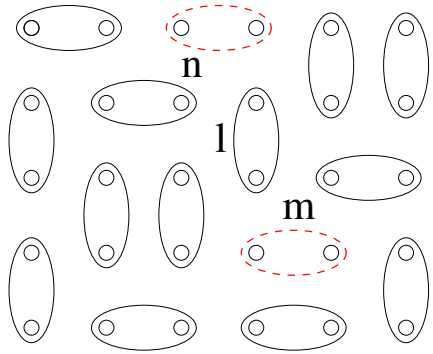

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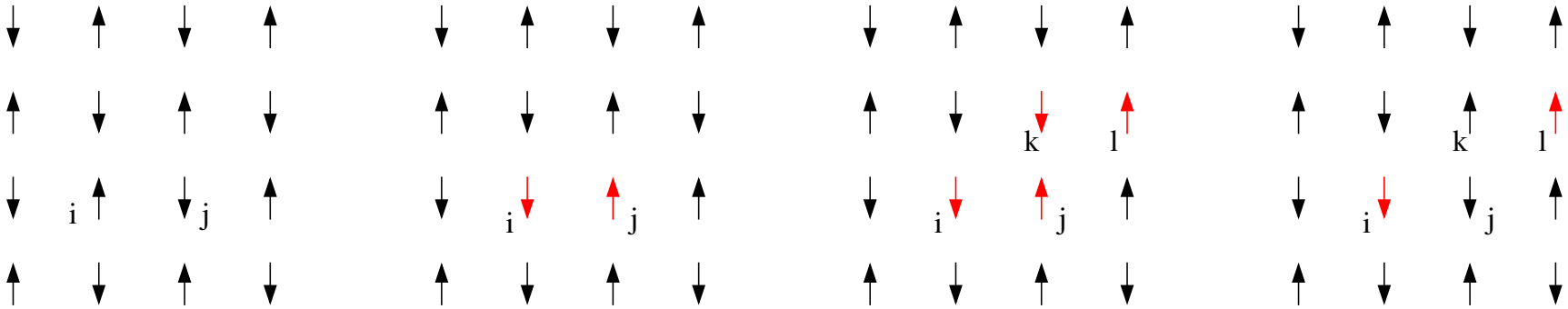
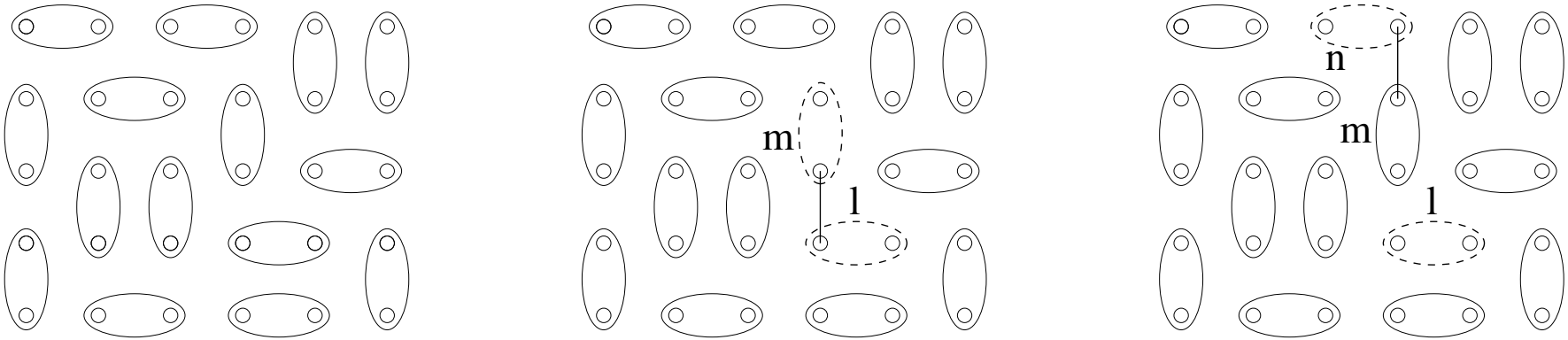
Excitations of the singlet soup

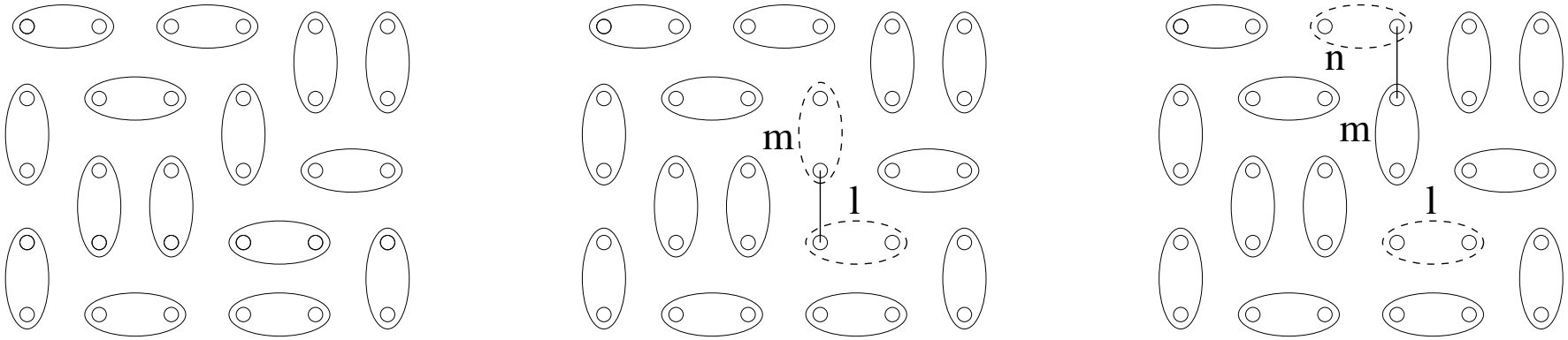
Now compare



and



Excitations of the singlet soup



- Assume that the dimers are labeled by $l, m, n \cdots \in \{1, 2, \ldots, \frac{N}{2}\}$
- Introduce Bosons which stand for a singlet or a triplet, created by $s_m^\dagger$ and $t_{m,\alpha}^\dagger$ $\alpha \in \{x, y, z\}$
- The first transition is described by $t_{m,x}^\dagger t_{l,x}^\dagger s_m s_l$ the second one by $t_{n,x}^\dagger s_m^\dagger t_{m,x} s_n$
- Why Bosons? Singlet and triplet consist of two electrons each so that operators referring to different dimers commute
- Next we need to set up the Hamiltonian for the Bosons

A technical detail

We found ($\alpha \in \{x, y, z\}$)

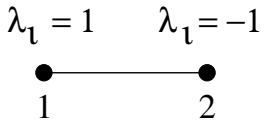
$$S_{1,\alpha}|s\rangle = \frac{1}{2}|t_\alpha\rangle \qquad S_{1,\alpha}|t_\alpha\rangle = \frac{1}{2}|s\rangle$$

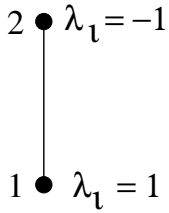
Now exchange $1 \leftrightarrow 2$

$$S_{2,\alpha}|s\rangle = -\frac{1}{2}|t_\alpha\rangle \qquad -S_{2,\alpha}|t_\alpha\rangle = \frac{1}{2}|s\rangle$$

Sign of matrix element depends on 'where the spin operator touches the dimer'

We need to adopt a convention how to label the sites in the dimers



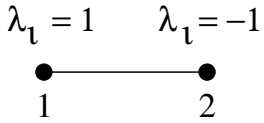


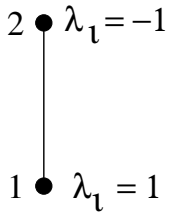
$$S_{i,\alpha}|s\rangle = \frac{\lambda_i}{2}|t_\alpha\rangle$$

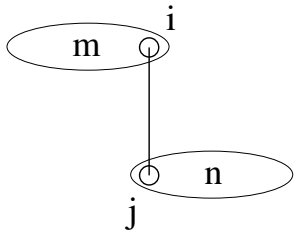
$$S_{i,\alpha}|t_\alpha\rangle = \frac{\lambda_i}{2}|s\rangle$$

Transcribing the Hamiltonian

- Spin operator: $\mathbf{S}_j \rightarrow \frac{\lambda_j}{2}\left(\mathbf{t}^\dagger s + s^\dagger \mathbf{t}\right) - \frac{i}{2}\,\mathbf{t}^\dagger \times \mathbf{t}$







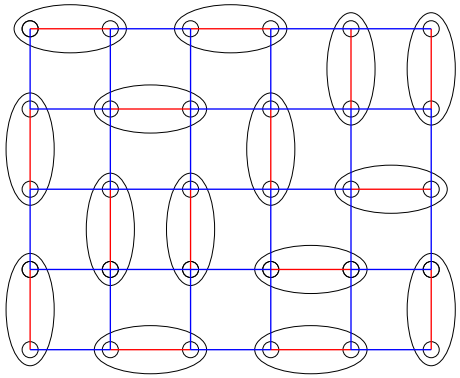
$$J\,\mathbf{S}_i \cdot \mathbf{S}_j \rightarrow \frac{J\lambda_i\lambda_j}{4}\left(s_m^\dagger \mathbf{t}_m + \mathbf{t}_m^\dagger s_m\right)\cdot\left(s_n^\dagger \mathbf{t}_n + \mathbf{t}_n^\dagger s_n\right) - \frac{J}{4}\left(\mathbf{t}_n^\dagger \times \mathbf{t}_n\right)\cdot\left(\mathbf{t}_m^\dagger \times \mathbf{t}_m\right)$$

$$-\frac{iJ}{4}\left[\lambda_i\left(s_m^\dagger \mathbf{t}_m + \mathbf{t}_m^\dagger s_m\right)\cdot\left(\mathbf{t}_n^\dagger \times \mathbf{t}_n\right) + \lambda_j\left(s_n^\dagger \mathbf{t}_n + \mathbf{t}_n^\dagger s_n\right)\cdot\left(\mathbf{t}_m^\dagger \times \mathbf{t}_m\right)\right]$$

This was for bonds which connect dimers - the exchange term within the dimers is

$$H_{intra} = \sum_m\left(\frac{J}{4}\,\mathbf{t}_m^\dagger \cdot \mathbf{t}_m - \frac{3J}{4}\,s_m^\dagger s_m\right) = J\sum_m \mathbf{t}_m^\dagger \cdot \mathbf{t}_m - \frac{N}{2}\,\frac{3J}{4}$$

All in all



$$H = J \sum_m \mathbf{t}_m^\dagger \cdot \mathbf{t}_m + \sum_{m,n} \left\{ \frac{J\lambda_i\lambda_j}{4} \left(s_m^\dagger \mathbf{t}_m + \mathbf{t}_m^\dagger s_m \right) \cdot \left(s_n^\dagger \mathbf{t}_n + \mathbf{t}_n^\dagger s_n \right) \right.$$

$$- \frac{iJ}{4} \left[\lambda_i \left(s_m^\dagger \mathbf{t}_m + \mathbf{t}_m^\dagger s_m \right) \cdot \left(\mathbf{t}_n^\dagger \times \mathbf{t}_n \right) + \lambda_j \left(s_n^\dagger \mathbf{t}_n + \mathbf{t}_n^\dagger s_n \right) \cdot \left(\mathbf{t}_m^\dagger \times \mathbf{t}_m \right) \right]$$

$$\left. - \frac{J}{4} \left(\mathbf{t}_n^\dagger \times \mathbf{t}_n \right) \cdot \left(\mathbf{t}_m^\dagger \times \mathbf{t}_m \right) \right\} - \mu \sum_m \left(\mathbf{t}_m^\dagger \cdot \mathbf{t}_m + s_m^\dagger s_m - 1 \right)$$

Constraint:

$$\mathbf{t}_m^\dagger \cdot \mathbf{t}_m + s_m^\dagger s_m = 1$$

Approximations start ...

$$J\,\mathbf{S}_i\cdot\mathbf{S}_j \;\rightarrow\; \frac{J\lambda_i\lambda_j}{4}\left(s_m^\dagger\mathbf{t}_m+\mathbf{t}_m^\dagger s_m\right)\cdot\left(s_n^\dagger\mathbf{t}_n+\mathbf{t}_n^\dagger s_n\right)-\frac{J}{4}\left(\mathbf{t}_n^\dagger\times\mathbf{t}_n\right)\cdot\left(\mathbf{t}_m^\dagger\times\mathbf{t}_m\right)$$
$$-\frac{iJ}{4}\left[\lambda_i\left(s_m^\dagger\mathbf{t}_m+\mathbf{t}_m^\dagger s_m\right)\cdot\left(\mathbf{t}_n^\dagger\times\mathbf{t}_n\right)+\lambda_j\left(s_n^\dagger\mathbf{t}_n+\mathbf{t}_n^\dagger s_n\right)\cdot\left(\mathbf{t}_m^\dagger\times\mathbf{t}_m\right)\right]$$

- First step: Assume singlet Bosons as condensed into the state with $\mathbf{k}=0$
- Replace the operators $s_m^\dagger$ and s_m by the (real) condensation amplitude s

$$J\,\mathbf{S}_i\cdot\mathbf{S}_j \;\rightarrow\; \frac{Js^2\lambda_i\lambda_j}{4}\left(\mathbf{t}_m+\mathbf{t}_m^\dagger\right)\cdot\left(\mathbf{t}_n+\mathbf{t}_n^\dagger\right)-\frac{J}{4}\left(\mathbf{t}_n^\dagger\times\mathbf{t}_n\right)\cdot\left(\mathbf{t}_m^\dagger\times\mathbf{t}_m\right)$$
$$-\frac{iJs}{4}\left[\lambda_i\left(\mathbf{t}_m+\mathbf{t}_m^\dagger\right)\cdot\left(\mathbf{t}_n^\dagger\times\mathbf{t}_n\right)+\lambda_j\left(\mathbf{t}_n+\mathbf{t}_n^\dagger\right)\cdot\left(\mathbf{t}_m^\dagger\times\mathbf{t}_m\right)\right]$$

This gives a quadratic term $\left(\mathbf{t}_m+\mathbf{t}_m^\dagger\right)\cdot\left(\mathbf{t}_n+\mathbf{t}_n^\dagger\right)=\mathbf{t}_m^\dagger\cdot\mathbf{t}_n+\mathbf{t}_n^\dagger\cdot\mathbf{t}_m+\mathbf{t}_m^\dagger\cdot\mathbf{t}_n^\dagger+\mathbf{t}_n\cdot\mathbf{t}_m$

Approximations continue ....

$$J\,\mathbf{S}_i\cdot\mathbf{S}_j \quad\rightarrow\quad \frac{Js^2\lambda_i\lambda_j}{4}\left(\mathbf{t}_m^\dagger\cdot\mathbf{t}_n+\mathbf{t}_n^\dagger\cdot\mathbf{t}_m+\mathbf{t}_m^\dagger\cdot\mathbf{t}_n^\dagger+\mathbf{t}_n\cdot\mathbf{t}_m\right)-\frac{J}{4}\,(\mathbf{t}_n^\dagger\times\mathbf{t}_n)\cdot(\mathbf{t}_m^\dagger\times\mathbf{t}_m)$$

$$-\frac{iJs}{4}\left[\lambda_i\left(\mathbf{t}_m+\mathbf{t}_m^\dagger\right)\cdot(\mathbf{t}_n^\dagger\times\mathbf{t}_n)+\lambda_j\left(\mathbf{t}_n+\mathbf{t}_n^\dagger\right)\cdot(\mathbf{t}_m^\dagger\times\mathbf{t}_m)\right]$$

The quartic term can be treated in mean-field approximation - however, it turns out that the corrections always are small

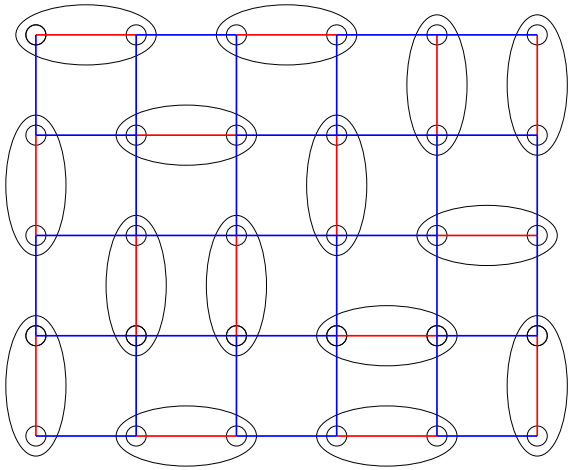
There remains the last line....this contain terms like $\mathbf{t}_m^\dagger\cdot(\mathbf{t}_n^\dagger\times\mathbf{t}_n)$ -

'one triplet in - two triplets out'

For phonons this would describe the 'decay' of a phonon due to anharmonicities

For simplicity we simply discard this term ....

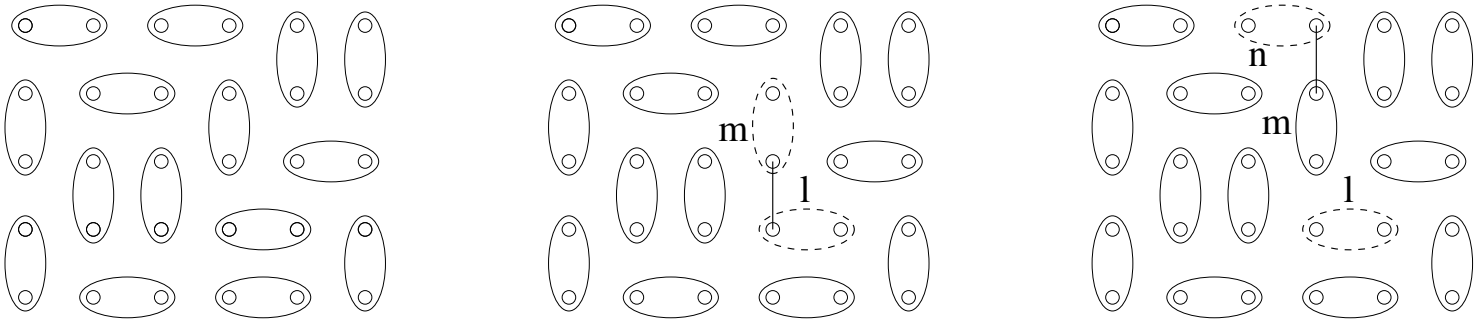
Approximate Hamiltonian



$$H = J \sum_m \mathbf{t}_m^\dagger \cdot \mathbf{t}_m + \sum_{i,j} \frac{J s^2 \lambda_i \lambda_j}{4} \left(\mathbf{t}_m^\dagger \cdot \mathbf{t}_n + \mathbf{t}_n^\dagger \cdot \mathbf{t}_m + \mathbf{t}_m^\dagger \cdot \mathbf{t}_n^\dagger + \mathbf{t}_m \cdot \mathbf{t}_n \right)$$

$$- \mu \sum_m \left(\mathbf{t}_m^\dagger \cdot \mathbf{t}_m + s^2 - 1 \right)$$

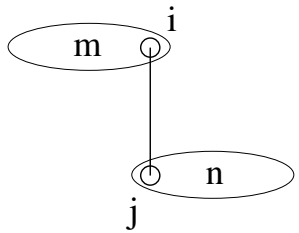
Final Approximation



- The excitations of the ‘singlet soup’ can be described as propagating triplets
- This seems to be of little use because there is no unique dimer covering and for a macroscopic system we cannot even write down a single one
- However, we can represent the Heisenberg exchange in terms of singlets and triplets for any dimer covering
- Therefore any dimer covering should give the same results
- Therefore we might come up with the idea to average the dimer Hamiltonian over all possible coverings

Averaging the dimer Hamiltonian

- We put a dimer on any of the $2N$ bonds of the lattice



- If two dimers m and n are connected by a term $\mathbf{S}_i \cdot \mathbf{S}_j$ the averaged Hamiltonian is

$$\bar{h}_{m,n} = \zeta \, h_{m,n} \qquad \zeta = \frac{N_{m,n}}{N_d}$$

$$h_{m,n} = \frac{Js^2 \lambda_i \lambda_j}{4} \left(\mathbf{t}_m^\dagger \cdot \mathbf{t}_n + \mathbf{t}_n^\dagger \cdot \mathbf{t}_m + \mathbf{t}_m^\dagger \cdot \mathbf{t}_n^\dagger + \mathbf{t}_m \cdot \mathbf{t}_n \right)$$

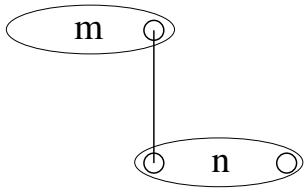
- $N_{m,n}$: Number of dimer coverings which contain the bonds n and m
- N_d: Total number of dimer coverings

Averaging the dimer Hamiltonian

We had

$$\bar{h}_{m,n} = \zeta \, h_{m,n} \qquad\qquad \zeta = \frac{N_{m,n}}{N_d}$$

We use a crude estimate for ζ



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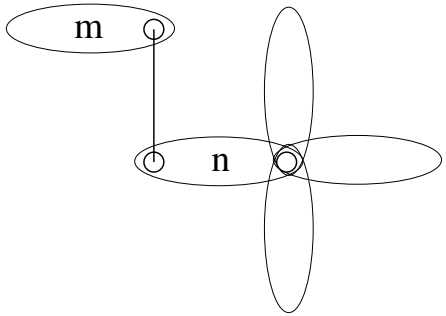

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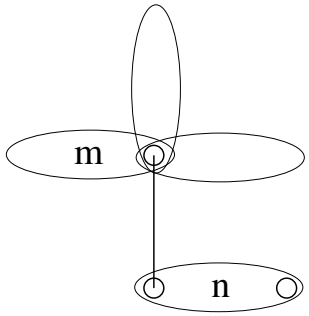


This gives $\zeta \approx \frac{1}{12}$

Final Hamiltonian

In this way we obtain the final triplet Hamiltonian ($J_{eff} = J - \mu$)

$$H = J_{eff} \sum_m \mathbf{t}_m^\dagger \cdot \mathbf{t}_m^\dagger + \frac{s^2\zeta}{4} \sum_{m\cap n=0} \sum_{\substack{i\in m \\ j\in n}} J_{i,j}\, \lambda_i \lambda_j \left(\mathbf{t}_m^\dagger \cdot \mathbf{t}_n^\dagger + \mathbf{t}_n \cdot \mathbf{t}_m + \mathbf{t}_m^\dagger \cdot \mathbf{t}_n + \mathbf{t}_n^\dagger \cdot \mathbf{t}_m \right)$$

- Sum over $m \cap n = 0$ runs over all nonintersecting pairs of bonds
- $J_{i,j} = J$ if i and j are nearest neighbors and zero otherwise
- H is a quadratic form and can be diagonalized by Fourier transform and Bosonic Bogoliubov transformation -see notes - and we obtain

$$\begin{aligned} \omega_{\mathbf{k}} &= \sqrt{J_{eff}^2 + 2J_{eff}\lambda_{\mathbf{k}}} \\ \lambda_{\mathbf{k}} &= s^2\zeta J \left(\frac{3}{2} + 2\gamma_{\mathbf{k}} - 4\gamma_{\mathbf{k}}^2 \right) \\ \gamma_{\mathbf{k}} &= \frac{1}{2} \left(cos(k_x) + \cos(k_y) \right) \end{aligned}$$

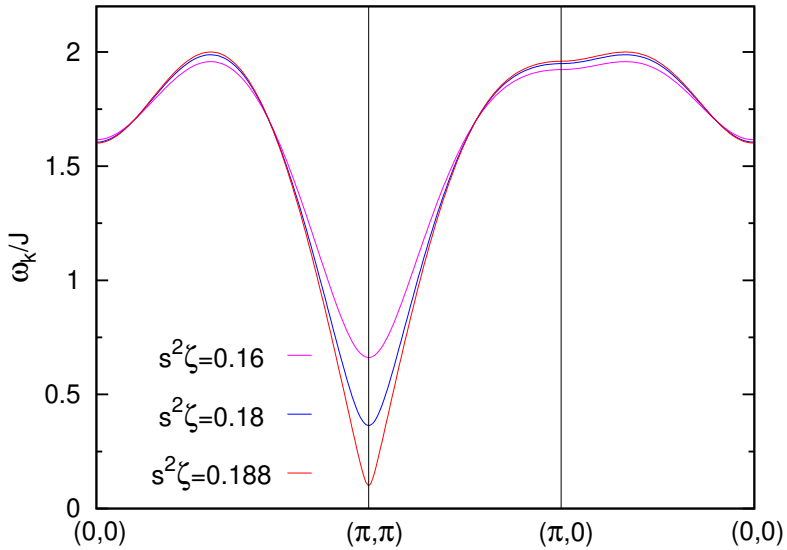
Recall:

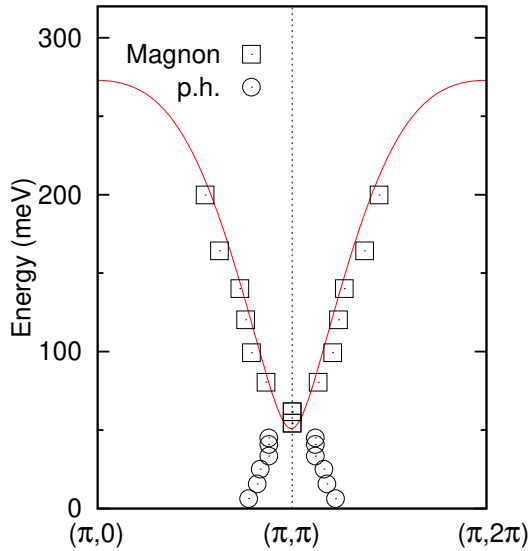
$$\omega_{\mathbf{k}} = \sqrt{J_{eff}^2 + 2J_{eff}\lambda_{\mathbf{k}}}$$

$$\lambda_{\mathbf{k}} = s^2\zeta J\left(\frac{3}{2} + 2\gamma_{\mathbf{k}} - 4\gamma_{\mathbf{k}}^2\right)$$

$$\gamma_{\mathbf{k}} = \frac{1}{2}\left(cos(k_x) + \cos(k_y)\right)$$

- We should now set up a self-consistency procedure to determine the renormalized triplet energy $J_{eff} = J - \mu$ and singlet condensation amplitude s^2
- However, we simplify matters and adjust the two unknown parameters J_{eff} and $s^2\zeta$ to reproduce two characteristic energies: bandwidth $2J$ and spin gap Δ_s





Doped Mott insulator

- We return to the single dimer but now consider the case of one electron

$$H = -t \sum_{\sigma} \left(\hat{c}^{\dagger}_{1,\sigma} \hat{c}_{2,\sigma} + \hat{c}^{\dagger}_{2,\sigma} \hat{c}_{1,\sigma} \right) + J\, \mathbf{S}_1 \cdot \mathbf{S}_2$$

- Only the term $\propto t$ can be active
- Its eigenstates are the bonding (+) and antibonding (-) state

$$|f_{\pm,\sigma}\rangle = \frac{1}{\sqrt{2}} (\hat{c}^{\dagger}_{1,\sigma} \pm \hat{c}^{\dagger}_{2,\sigma})|0\rangle$$

- They have spin $\sigma = \pm\frac{1}{2}$ - the spin quantum numbers of an electron
- They have energy $-t$ (bonding) and t (antibonding)
- We incorporate these into our theory by introducting a new type of bond particle
- If dimer m is in one of the states $|f_{\pm,\sigma}\rangle$ we consider it as occupied by a Fermion, created by $f^{\dagger}_{m,\pm,\sigma}$
- Why a Fermion? Because these states have an odd number of electrons!

Transcribing the Fermion operator

The two Fermion creation/annihilaton operators can be combined into a spinor

$$\mathbf{c}^\dagger = \begin{pmatrix} c_\uparrow^\dagger \\ c_\downarrow^\dagger \end{pmatrix} \qquad \mathbf{c} = \begin{pmatrix} c_\uparrow \\ c_\downarrow \end{pmatrix}$$

- Under spin rotations $\mathbf{c}$ transforms like $i\tau_y \mathbf{c}^\dagger$ ($i\tau_y$ is the 'metric spinor')
- The representation of the $\mathbf{c}_j$-spinor is found to be

$$\mathbf{c}_j \quad \rightarrow \quad \frac{1}{2} \; : \; \left(s \, i\tau_y + \lambda_j \, \mathbf{t} \cdot \vec{\tau} \, i\tau_y \right) \left(\mathbf{f}_+^\dagger - \lambda_j \, \mathbf{f}_-^\dagger \right) \; :$$

- s and $\mathbf{t}$ are the annihilation operators for singlet and triplet Bosons
- $\vec{\tau}$ is the vector of Pauli matrices
- The 'spinor product' $\mathbf{t} \cdot \vec{\tau} \, i\tau_y \, \mathbf{f}^\dagger$ is how to construct a spinor from a vector operator and a spinor - i.e. familiar angular momentum addition

Doped Holes

$$\mathbf{c}_j \rightarrow \frac{1}{2}\left(s\, i\tau_y + \lambda_j\, \mathbf{t}\cdot\vec{\tau}\, i\tau_y\right)\left(\mathbf{f}_+^\dagger - \lambda_j\, \mathbf{f}_-^\dagger\right)$$

$$\mathbf{c}_i^\dagger \rightarrow \frac{1}{2}\left(s^\dagger\, i\tau_y + \lambda_i\, \mathbf{t}^\dagger\cdot\vec{\tau}\, i\tau_y\right)\left(\mathbf{f}_+ - \lambda_i\, \mathbf{f}_-\right)$$

- From here on everything is analogous to the procedure for triplets
- We 'translate' $-t\sum_\sigma \hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma}$ - this gives a complicated expression ...
- We again simplify this by replacing the singlet operators s_m and $s_m^\dagger$ by the condensation amplitude s and dropping the triplets
- We again do the averaging over dimer coverings thereby introducing ζ
- In the end we again obtain a Hamiltonian which is a quadratic form
- The lowest hole-band becomes

$$\epsilon_{\mathbf{k}} = const + 2s^2\zeta t(\gamma_{\mathbf{k}} + 2\gamma_{\mathbf{k}}^2)$$

- However, we need to discuss how to determine the Fermi surface

Counting electrons

- The constraint now becomes

$$s_m^\dagger s_m + \mathbf{t}_m^\dagger \cdot \mathbf{t}_m + \sum_\sigma \left(f_{m,+,\sigma}^\dagger f_{m,+,\sigma} + f_{m,-,\sigma}^\dagger f_{m,-,\sigma} \right) = 1$$

- For a fixed dimer covering the number of electrons is

$$\begin{aligned} N_e &= 2 \cdot \sum_m \left(s_m^\dagger s_m + \mathbf{t}_m^\dagger \cdot \mathbf{t}_m \right) + 1 \cdot \sum_{m,\sigma} \left(f_{m,+,\sigma}^\dagger f_{m,+,\sigma} + f_{m,-,\sigma}^\dagger f_{m,-,\sigma} \right) \\ &= 2 \cdot \sum_m \left(s_m^\dagger s_m + \mathbf{t}_m^\dagger \cdot \mathbf{t}_m + \sum_\sigma \left(f_{m,+,\sigma}^\dagger f_{m,+,\sigma} + f_{m,-,\sigma}^\dagger f_{m,-,\sigma} \right) \right) \\ &\qquad -1 \cdot \sum_{m,\sigma} \left(f_{m,+,\sigma}^\dagger f_{m,+,\sigma} + f_{m,-,\sigma}^\dagger f_{m,-,\sigma} \right) \\ &= 2 \cdot \frac{N}{2} - \sum_{m,\sigma} \left(f_{m,+,\sigma}^\dagger f_{m,+,\sigma} + f_{m,-,\sigma}^\dagger f_{m,-,\sigma} \right) \end{aligned}$$

We had

$$
\begin{aligned}
N_e &= N - \sum_{m,\sigma} \left(f^\dagger_{m,+,\sigma} f_{m,+,\sigma} + f^\dagger_{m,-,\sigma} f_{m,-,\sigma} \right) \\
1-\delta &= 1 - \frac{1}{N} \sum_{m,\sigma} \left(f^\dagger_{m,+,\sigma} f_{m,+,\sigma} + f^\dagger_{m,-,\sigma} f_{m,-,\sigma} \right) \\
\delta &= \frac{1}{N} \sum_{m,\sigma} \left(f^\dagger_{m,+,\sigma} f_{m,+,\sigma} + f^\dagger_{m,-,\sigma} f_{m,-,\sigma} \right)
\end{aligned}
$$

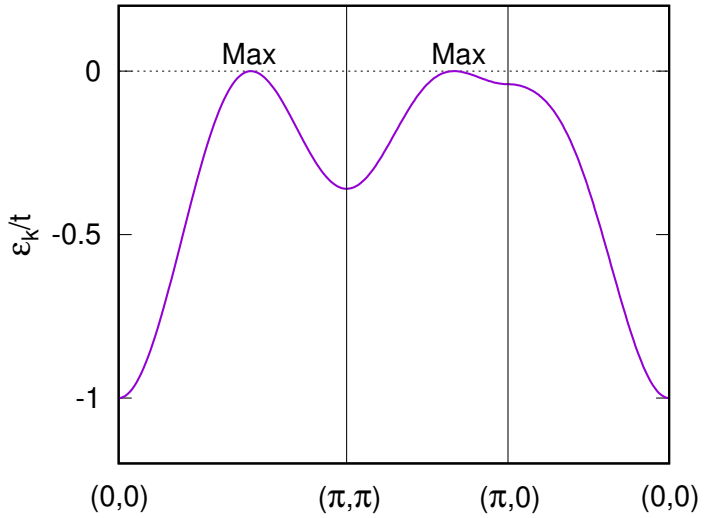
- The doped holes correspond to spin-$\frac{1}{2}$ Fermions - compare Hubbard-I
- The Fermi surface is a hole pocket whose area is $\propto \delta$
- When approaching the Mott insulator - $\delta \to 0$ - the area of the hole pocket shrinks to zero

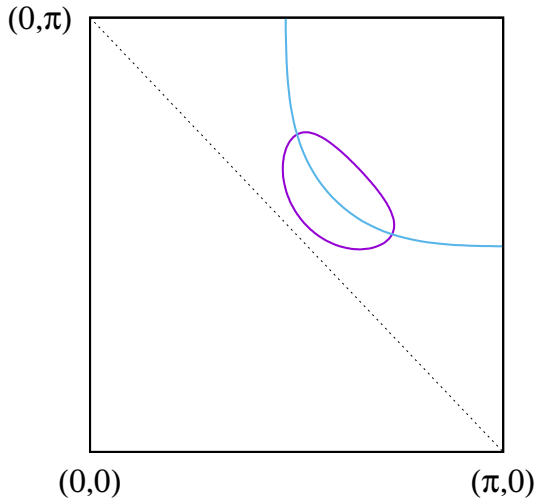
Bands and Fermi surface

The topmost band for the Fermions

$$\epsilon_{\mathbf{k}} = const + 2s^2\zeta t(\gamma_{\mathbf{k}} + 2\gamma_{\mathbf{k}}^2)$$

With $s^2\zeta = 0.16$:

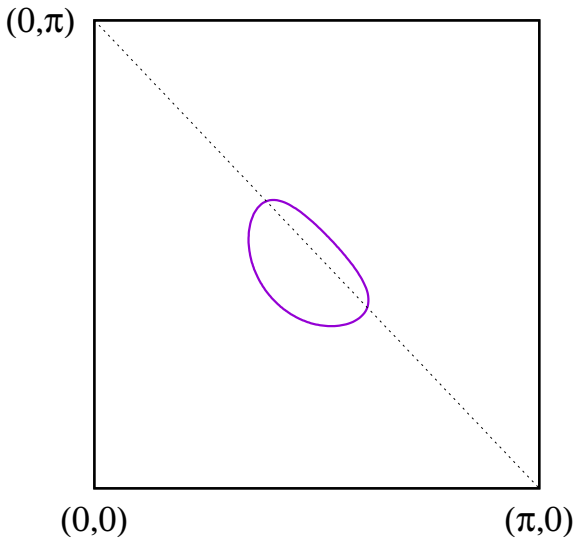




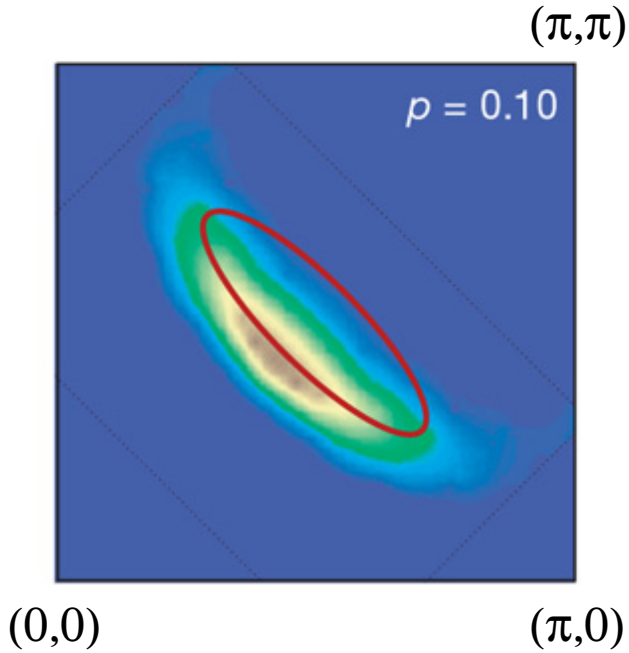
- With hopping terms between $(1,1)$- and $(2,0)$-like neighbors the Fermi surface becomes a hole pocket
- Here $t' = -0.2t$, $t'' = 0.1t$, $\delta = 0.1$

Comparison to experiment

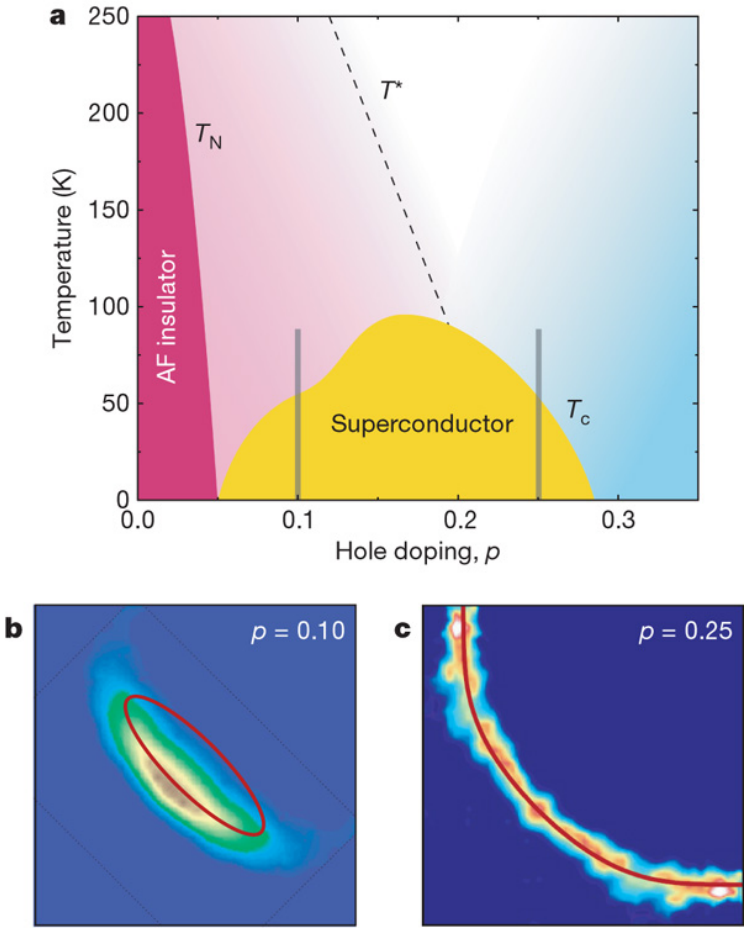
FS from dimer theory - with shift

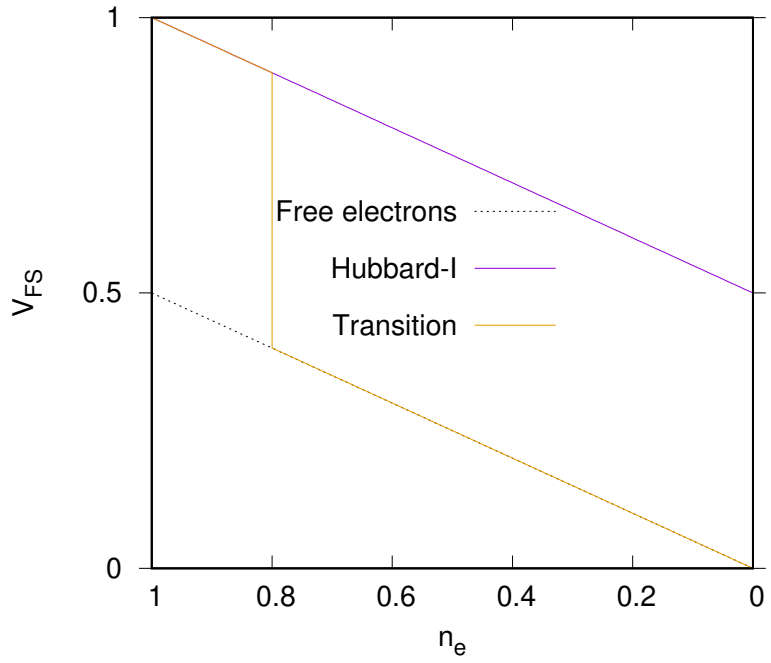


FS in the ‘pseudogap phase’



Phase diagram revisited





Summary

- The goal of the lecture was mainly to show why doped Mott insulator are so tough to handle
- The two Hubbard bands must be in the theory from the very beginning - only the Hubbard-I approximations and extensions do this
- The ions in a Mott insulator carry a spin - the spins ‘communicate’ resulting in spin excitations
- Mobile carriers interact strongly with spin excitations resulting in massive modification of the band structure
- While much of this can be treated in an antiferromagnetic state the state showing superconductivity has no order
- Finally another key problem is how to describe the phase transition small Fermi surface to large Fermi surface