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The physics of doped Mott insulators

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Mott insulators

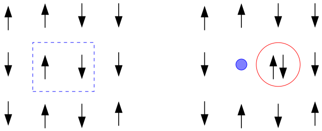
The simplest model to describe Mott insulators is the Hubbard model (see lecture by E. Pavarini)

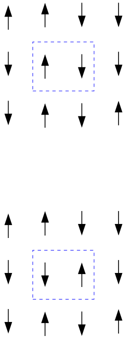
$$H = -t \sum_{\langle i,j \rangle} \sum_{\sigma} \left(c^{\dagger}_{i,\sigma} c_{j,\sigma} + c^{\dagger}_{j,\sigma} c_{i,\sigma} \right) + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow}$$

- We consider this model on a 2D square lattice with N sites
- $< i,j >$ denotes sum over all $2N$ pairs of nearest neighbors
- Hopping between more distant neighbors could be included but for the time being we omit this
- We assume $U/t \gg 1$
- Initially number of electrons $N_e = N$ or one electron per site
- Electron density is denoted by $n_e = N_e/N = 1$

Mott insulators

We recall U/t is finite but $U/t \gg 1$





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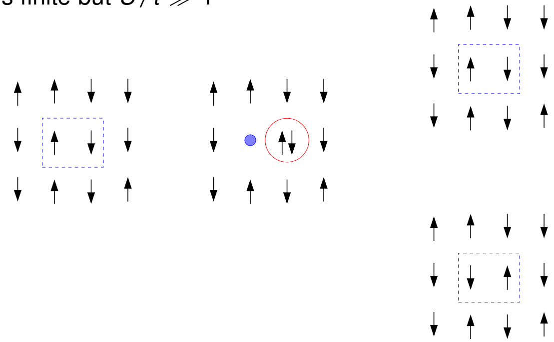


- By processes like this the spins can ‘communicate’ with one another
- It is energetically favourable if two spins on neighboring sites are antiparallel
- Two opposite spins on neighboring sites can simultaneously flip their direction

Mott insulators

The Mott-insulator with finite U/t is described by the Heisenberg antiferromagnet

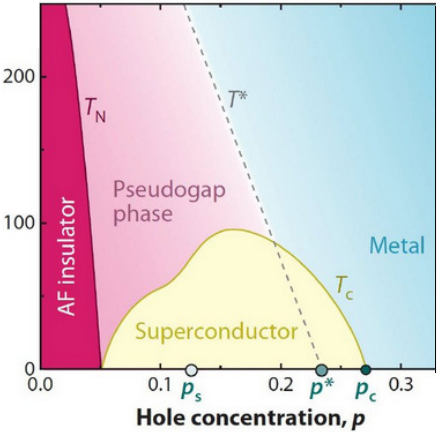
$$
\begin{aligned}
H &= J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j \\
&= J \sum_{\langle i,j \rangle} \left(\quad S_i^x S_j^x + S_i^y S_j^y \quad + S_i^z S_j^s \right) \\
&= J \sum_{\langle i,j \rangle} \left(\frac{1}{2} \left(S_i^+ S_j^- + S_i^- S_j^+ \right) + S_i^z S_j^z \right)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

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

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

Doped Mott insulators

A Mott insulator is not that spectacular - to observe spectacular phenomena such as high-temperature the electron density has to be reduced $n_e \to 1 - p$



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

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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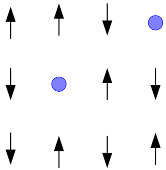

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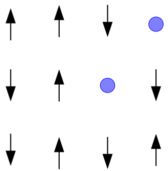

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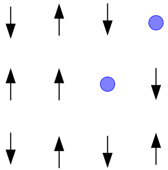

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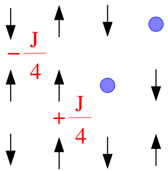

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The t-J model

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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 $t \approx 350$meV and $J \approx 140$meV, so $J/t = 0.4$

The Heisenberg antiferromagnet

We consider the case $N_e = N$ - one electron/site $\Rightarrow$ no hopping is possible

Only the spin exchange (Heisenberg antiferromagnet) is active

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

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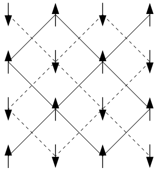
If only the term $\propto S_i^z \, S_j^z$ were present the ground state would be the Néel state



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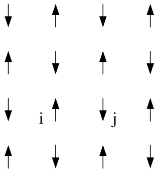

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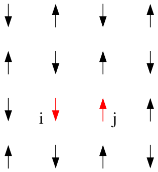

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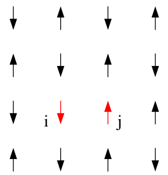

The Néel state is not an eigenstate of the full Hamiltonian because the term

$\propto S_i^+ \, S_j^- + S_i^- \, S_j^+$ produces quantum fluctuations

Linear spin wave theory

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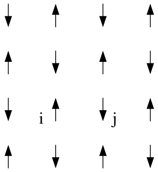
More on quantum fluctuations:



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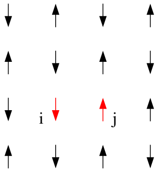

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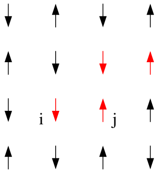

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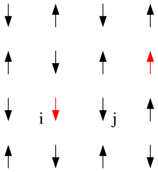

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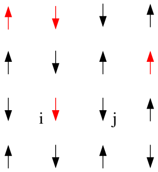

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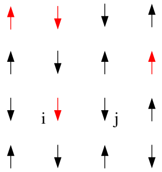
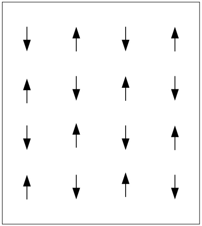
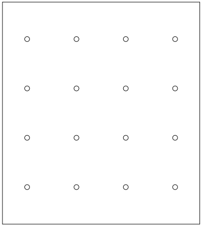


- There are two possible outcomes
- The quantum fluctuations could completely destroy the antiferromagnetic order and a qualitatively new state may ensue
- Or an equilibrium concentrations of inverted spins may be reached and we have an antiferromagnet hosting a gas of magnons
- In one dimension the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

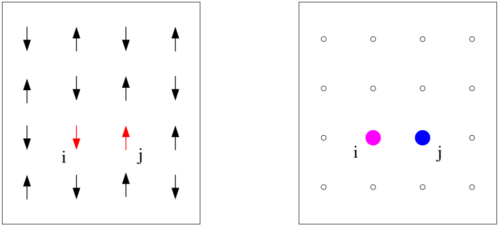
Linear spin wave theory





- Consider the Néel state as vacuum $|0\rangle$

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 $a_i^\dagger$
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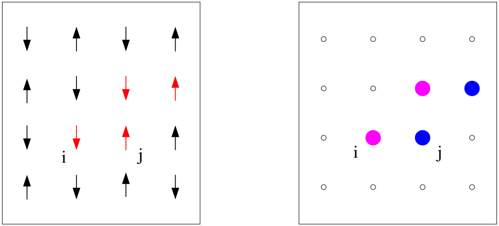
Linear spin wave theory



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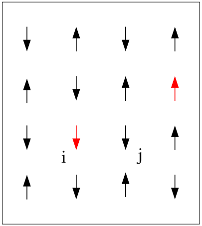

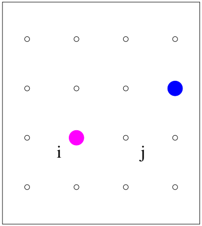

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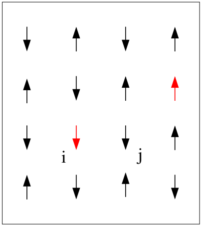

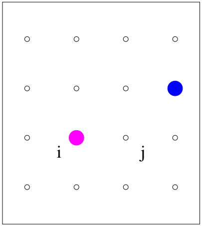

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- Why Bosons? - Spin operators on different sites commute!
- States like $(a_i^\dagger)^2|0\rangle$ are meaningless
- Additional constraint: at most one Boson/site - ‘hard core constraint’

Translating the Hamiltonian

- Represent a $\downarrow$-spin at site i on the $\uparrow$-sublattice as a Boson created by $a_i^\dagger$
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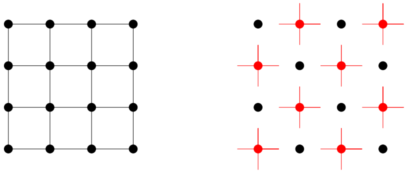
$$J \sum_{\langle i,j \rangle} \frac{1}{2} \left(S_i^- \; S_j^+ + S_i^+ \; S_j^- \right) = \frac{J}{2} \sum_{i \in \uparrow - SL} \sum_{j \in N(i)} \left(S_i^- \; S_j^+ + S_j^- \; S_i^+ \right)$$

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



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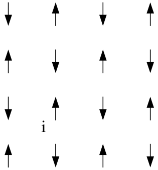

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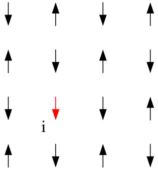

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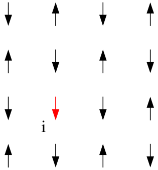

- An inverted spin is parallel rather than antiparallel to its $z = 4$ neighbors
- For $z = 4$ bonds the energy increases from $-\frac{J}{4}$ to $\frac{J}{4}$
- The total increase of energy is $\frac{zJ}{2}$
- We interpret this as the energy of the boson

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

Translating the Hamiltonian

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Collecting everything we find the spin wave Hamiltonian

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

Translating the Hamiltonian

Collecting everything we find the spin wave Hamiltonian

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We switch to Fourier transformed operators ...

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

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... and find

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

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

Bosonic Bogoliubov transformation

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

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

$$\alpha^\dagger_{\mathbf{k}} = u_{\mathbf{k}} \; a^\dagger_{\mathbf{k}} + v_{\mathbf{k}} \; b_{-\mathbf{k}},$$
$$\beta^\dagger_{-\mathbf{k}} = u_{\mathbf{k}} \; b^\dagger_{-\mathbf{k}} + v_{\mathbf{k}} \; a_{\mathbf{k}},$$

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

$$\left[\alpha_{\mathbf{k}}, \alpha^\dagger_{\mathbf{k}'}\right] = \left[\beta_{\mathbf{k}}, \beta^\dagger_{\mathbf{k}'}\right] = \delta_{\mathbf{k},\mathbf{k}'}$$

$$\left[H_{SW}, \alpha^\dagger_{\mathbf{k}}\right] = \omega_{\mathbf{k}} \; \alpha^\dagger_{\mathbf{k}}$$

Bosonic Bogoliubov transformation

This gives $|u_{\mathbf{k}}|^2 - |v_{\mathbf{k}}^2| = 1$ and the non-Hermitean eigenvalue problem ...

$$\frac{zJ}{2}\begin{pmatrix} 1 & -\gamma_{\mathbf{k}} \\ \gamma_{\mathbf{k}} & -1 \end{pmatrix}\begin{pmatrix} u_{\mathbf{k}} \\ v_{\mathbf{k}} \end{pmatrix} = \omega_{\mathbf{k}}\begin{pmatrix} u_{\mathbf{k}} \\ v_{\mathbf{k}} \end{pmatrix}.$$

... see my notes for details

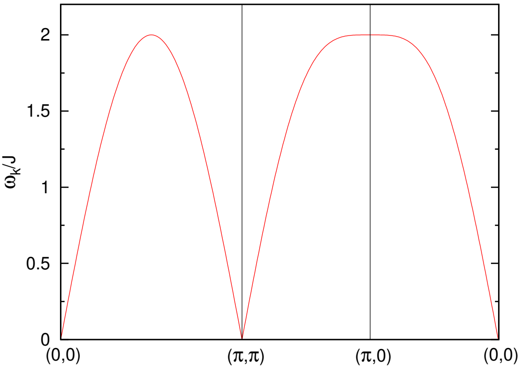
The characteristic equation can be easyly written down and gives the magnon dispersion

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

Spin waves or magnons

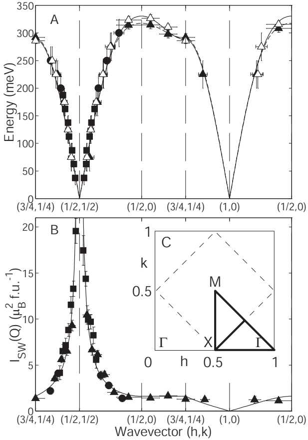
We found

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



Magnons are observed experimentally!

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 ...

... electrons in a Mott-insulator retain only their spin degrees of freedom

The spin degeneracy must be somehow resolved in that the spins arrange in some ‘pattern’

Deviations from this ‘pattern’ can aquire the character of Bosonic particles:
spin excitations

Mobile holes move through this ‘pattern’ and this drastically modifies their motion - as we will see now

Hole in an antiferromagnet

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

In this case the hopping term can act and we must consider the full t-J model

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

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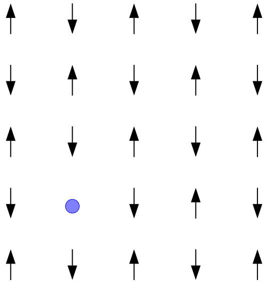
A single hole will not affect the magnetic order $\Rightarrow$ we start from the Néel state



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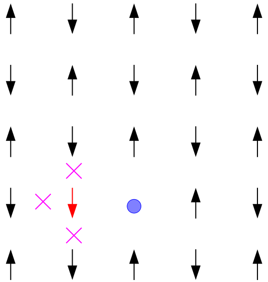

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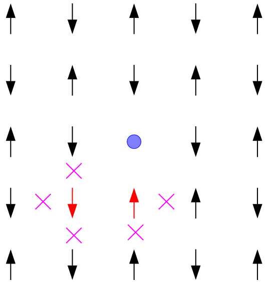

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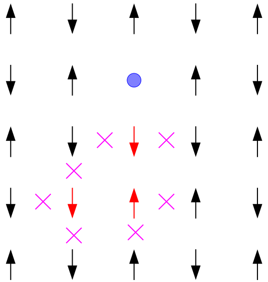

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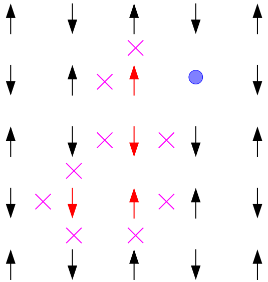

Hole in an antiferromagnet

The hole leaves behind a 'trace of frustration' - the magnetic energy increases linearly with the number of steps that the hole has taken

The hole is self-trapped

Hole in an antiferromagnet

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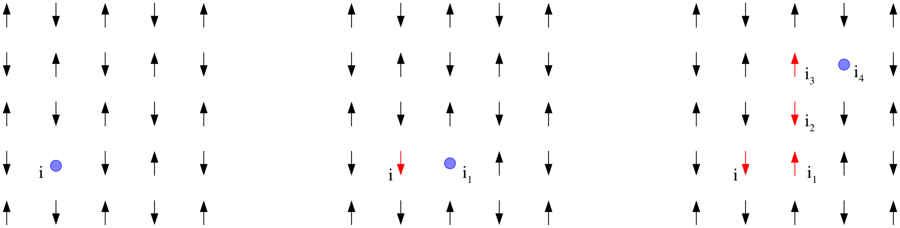
The hole is self-trapped

To find the resulting localized state we make the following ansatz

$$|\Phi_i\rangle = \sum_{\nu=0}^{\infty} \alpha_\nu \sum_{i_1,i_2,\ldots,i_\nu} |i, i_1, i_2, \ldots, i_\nu\rangle,$$



Hole in an antiferromagnet

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Our ansatz:

$$|\Phi_i\rangle = \sum_{\nu=0}^{\infty} \alpha_\nu \sum_{i_1, i_2, \ldots, i_\nu} |i, i_1, i_2, \ldots, i_\nu\rangle$$

We call the $|i, i_1, i_2, \ldots, i_\nu\rangle$ string states

We decompose the t-J Hamiltonian as ...

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

... and choose $H_0 = H_t + H_I$

We determine the coefficients α_ν variationally

$$E_{loc} = \frac{\langle \Phi_i | H_0 | \Phi_i \rangle}{\langle \Phi_i | \Phi_i \rangle} \rightarrow min$$

Hole in an antiferromagnet

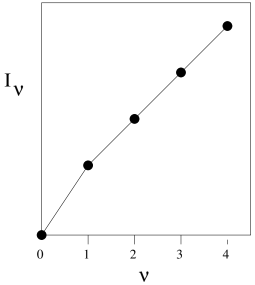
Performing the variational procedure (see notes for details) gives an eigenvalue problem

$$-\left(\tilde{t}_\nu \beta_{\nu+1} + \tilde{t}_{\nu-1}\beta_{\nu-1}\right) + I_\nu \beta_\nu \quad = \quad E_{loc}\,\beta_\nu$$

with the side condition $\beta_{-1} = 0$ - moreover

$$\beta_\nu \quad = \quad \sqrt{z(z-1)^{\nu-1}}\,\alpha_\nu$$

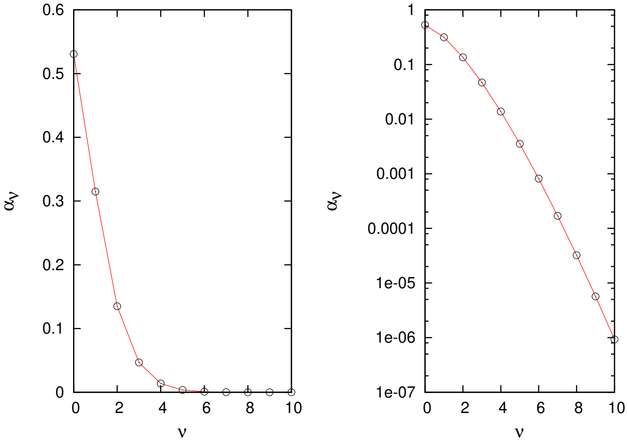
$$\tilde{t}_\nu \quad = \quad \begin{cases} \sqrt{z} & t \quad \nu = 0 \\ \sqrt{z-1} & t \quad \nu > 0 \end{cases}$$



Numerical solution gives β_ν and α_ν

Hole in an antiferromagnet

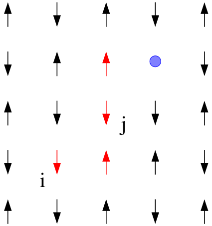
This is what the solution looks like for $J/t = 0.4$



Hole in an antiferromagnet

So far we find the hole is self-trapped...

However, at this point the part $H_\perp = \frac{J}{2} \sum_{\langle i,j \rangle} (S_i^+ S_j^- + H.c.)$ comes into play



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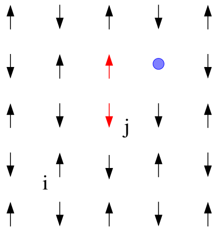

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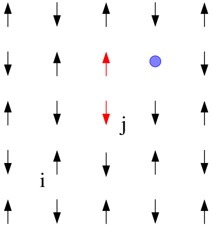
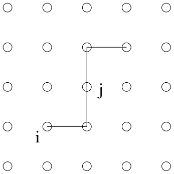


A string of length ν - coefficient α_ν is converted into one length $\nu \pm 2$ - coefficient $\alpha_{\nu\pm2}$ - described by the matrix element

$$\delta \left\langle \Phi_j | H_\perp | \Phi_i \right\rangle \quad = \quad J \sum_{\nu=0}^{\infty} (z-1)^\nu \alpha_\nu \alpha_{\nu+2} = J \cdot m$$

Hole in an antiferromagnet

One more detail



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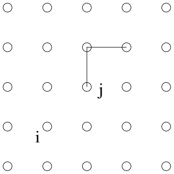

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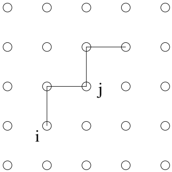

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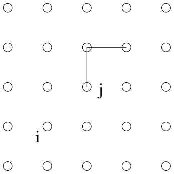

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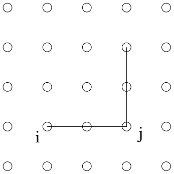

Hole in an antiferromagnet

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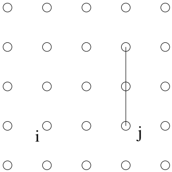

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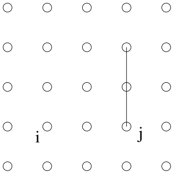

The matrix element to $(1, 1)$-like neighbors is twice that to $(2, 0)$-like

Hole in an antiferromagnet

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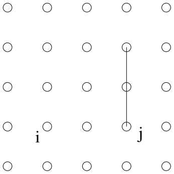
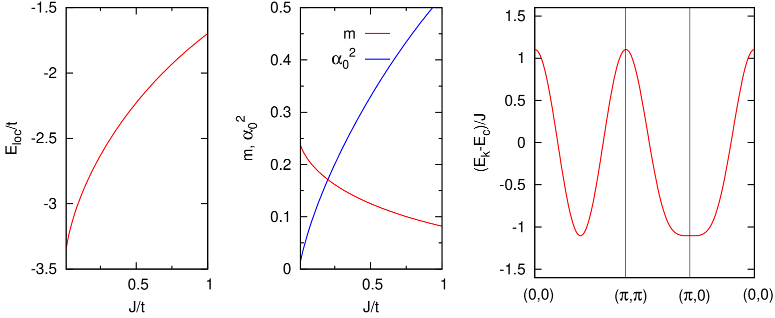


The matrix element to $(1,1)$-like neighbors is twice that to $(2,0)$-like neighbors

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

Hole in an antiferromagnet

Summary of results

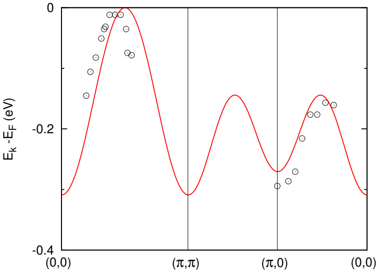


Note in particular: the bandwidth is $W \approx 2J$ - the free bandwidth would be

$W_{free} = 8t$ so that $\frac{W_{free}}{W} = \frac{4t}{J} = 10$ for $J/t = 0.4$

Hole in an antiferromagnet

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’ - they somehow arrange themselves to optimize the exchange energy $\propto J$ and deviations from this arrangement form a new type of excitations - spin excitations
- The holes move through this spin arrangement and their motion is modified by this - as we have just seen!

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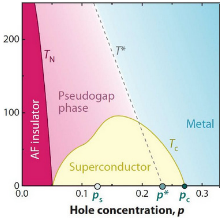
- The Heisenberg exchange gives the spins a 'life of their own' - they somehow arrange themselves to optimize the exchange energy $\propto J$ and deviations from this arrangement form a new type of excitations - spin excitations
- The holes move through this spin arrangement and their motion is modified by this - as we have just seen!
- For a finite concentration of holes this also goes the other way round - the spins are 'stirred' by the holes and modify their arrangement to some degree to accomodate the holes
- In fact in cuprate superconductors the Néel order disappears for hole concentrations of a few percent



Prelude: Dimer basis

We consider the t-J Hamiltonian on a dimer with sites labeled 1 and 2

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

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Combining everything

$$\mathbf{S}^2 = \mathbf{S}_1^2 + 2\, \mathbf{S}_1 \cdot \mathbf{S}_2 + \mathbf{S}_2^2 = S(S+1) \quad \Rightarrow \quad J\, \mathbf{S}_1 \cdot \mathbf{S}_2 = J \left(\frac{S(S+1)}{2} - \frac{3}{4} \right)$$

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Singlet and triplet are eigenstates of H with energies $-\frac{3J}{4}$ and $\frac{J}{4}$

Dimer basis

Singlet and triplet are eigenstates of H with energies $-\frac{3J}{4}$ and $\frac{J}{4}$

The wave functions are obtained by standard angular momentum coupling

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

- $|s\rangle$ the singlet and $|t_x\rangle$, $|t_y\rangle$ and $|t_z\rangle$ the three components of the triplet
- They are not eigenstates of S_z but are constructed to obey $S_\alpha |t_\beta\rangle = i\epsilon_{\alpha\beta\gamma} |t_\gamma\rangle$
- This means they behave like the three components of a vector under spin rotations

Dimer basis

We consider the effect of inversion I: $1 \leftrightarrow 2$

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

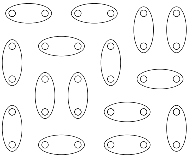
The singlet is even under inversion

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

The triplets are odd - the triplets have an ‘orientation’

Spin liquid

- 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 a product state

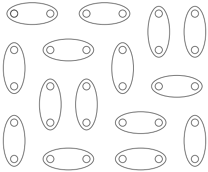
$$|\Psi_0\rangle = \prod_{(i,j)\in D} \frac{1}{\sqrt{2}} \left(c^\dagger_{i,\uparrow} c^\dagger_{j,\downarrow} - c^\dagger_{i,\downarrow} c^\dagger_{j,\uparrow} \right) |0\rangle$$

- 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' $H_d = J \sum_{(i,j)\in D} \mathbf{S}_i \cdot \mathbf{S}_j$

Spin liquid

Karlsruhe Institute of Technology

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



Spin liquid

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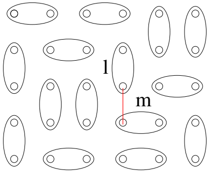

Let us assume we act with - say - $J\, S^x_i\, S^x_j$ along a bond not included in D

Spin liquid

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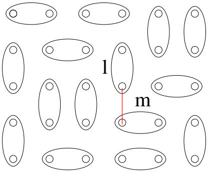

Let us assume we act with - say - $J\, S^x_i\, S^x_j$ along a bond not included in D

$$S_{1,x}|s\rangle = \frac{1}{2}\left(S_1^- + S_1^+\right) \frac{1}{\sqrt{2}} \left(c^\dagger_{1,\uparrow} c^\dagger_{2,\downarrow} - c^\dagger_{1,\downarrow} c^\dagger_{2,\uparrow} \right) |0\rangle$$

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

Spin liquid

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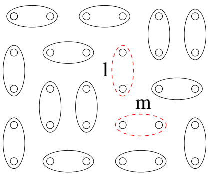

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Spin liquid

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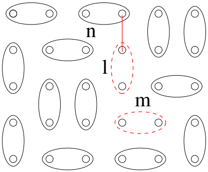

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Spin liquid

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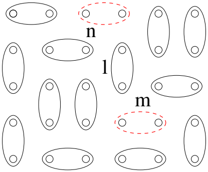

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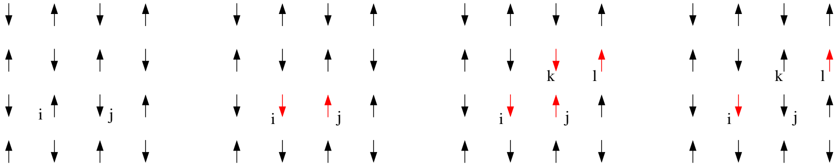
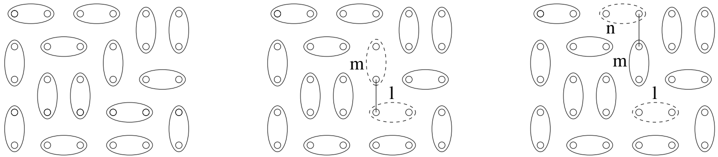
$$= \frac{1}{2\sqrt{2}} \left(c^\dagger_{1,\uparrow} c^\dagger_{2,\downarrow} - c^\dagger_{1,\downarrow} c^\dagger_{2,\uparrow} \right) |0\rangle = \frac{1}{2}\, |s\rangle$$

Spin liquid

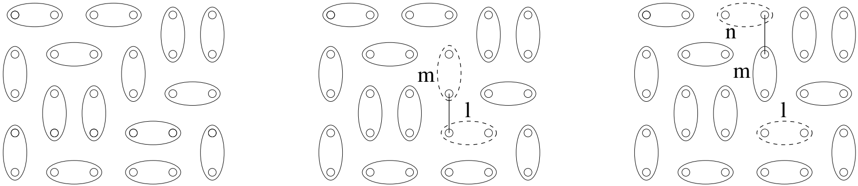
Now compare



and



Spin liquid



- We assume that the dimers are labeled by $m, n \in \{1, 2, \ldots, \frac{N}{2}\}$
- We 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

Spin liquid

We have already shown ($\alpha \in \{x, y, z\}$)

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

Spin liquid

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Now exchange $1 \leftrightarrow 2$

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

Spin liquid

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When a dimer is converted from singlet to triplet or vice versa the sign depends on ‘where the spin operator touches the dimer’

Spin liquid

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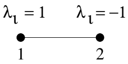
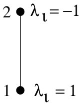
When a dimer is converted from singlet to triplet or vice versa the sign depends on 'where the spin operator touches the dimer'

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

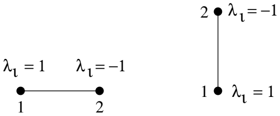




$$S_{i,\alpha}|s\rangle = \frac{\lambda_i}{2}\,|t_\alpha\rangle$$
$$S_{i,\alpha}|t_\alpha\rangle = \frac{\lambda_i}{2}\,|s\rangle$$

Spin liquids

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



Spin liquids

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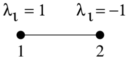
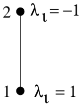
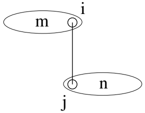




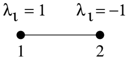


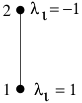
$$J\,\mathbf{S}_i \cdot \mathbf{S}_j \quad \rightarrow \quad \frac{J\lambda_i\lambda_j}{4}\left(s_m^\dagger \mathbf{t}_m + \mathbf{t}_m^\dagger s_m\right) \cdot \left(s_n^\dagger \mathbf{t}_n + \mathbf{t}_n^\dagger s_n\right) - \frac{J}{4}\,(\mathbf{t}_n^\dagger \times \mathbf{t}_n) \cdot (\mathbf{t}_m^\dagger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

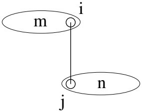
$$-\frac{iJ}{4}\left[\lambda_i \left(s_m^\dagger \mathbf{t}_m + \mathbf{t}_m^\dagger s_m\right) \cdot (\mathbf{t}_n^\dagger \times \mathbf{t}_n) + \lambda_j \left(s_n^\dagger \mathbf{t}_n + \mathbf{t}_n^\dagger s_n\right) \cdot (\mathbf{t}_m^\dagger \times \mathbf{t}_m)\right]$$

Spin liquids

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







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

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

To make things even worse this has to be solved under the constraint

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

Spin liquids

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

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Spin liquids

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First - and crucial - step of simplification: consider singlets as ‘inert background’

Spin liquids

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First - and crucial - step of simplification: consider singlets as ‘inert background’

We consider singlet Bosons as condensed into the state with $\mathbf{k}=0$

Then we can replace the operators $s_m^\dagger$ and s_m by a (real) number s

Spin liquids

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

Spin liquids

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

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

Spin liquid

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

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

Spin liquid

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

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

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

Spin liquid

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

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

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

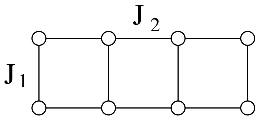
For simplicity we discard this term....

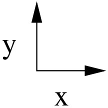
We have seen that ...

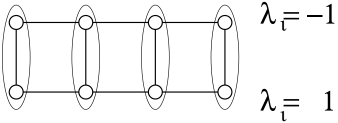
- ... we can write down a theory for a disordered spin system by starting from a ‘singlet soup’
- This is - essentially - the only known way of writing down a wave function which obeys the constraint of having one spin per site, has no order and is a singlet
- The excitations of the ‘singlet soup’ are triplet-excited dimers which can propagate
- We were forced to make quite some approximations
- To illustrate its usefulness and further develop the theory we now apply it to spin ladders following the seminal work of Gopalan, Rice, and Sigrist, PRB **49**, 8901 (1994)

Spin ladders

In compounds such as $SrCu_2O_3$ the spins are arranged like this







Two successive rungs m and $m+1$ are connected by two exchange bonds

The product $\lambda_i \lambda_j$ is always 1 - the contributions add up

The 'anharmonic term' contains only one factor of λ - the contributions cancel

With our simplifications we get $H = H_1 + H_2$

$$H_0 = \sum_m \left(-\frac{3J_1}{4} s_m^\dagger s_m + \frac{J_1}{4} \mathbf{t}_m^\dagger \cdot \mathbf{t}_m \right) \rightarrow J_1 \sum_m \mathbf{t}_m^\dagger \cdot \mathbf{t}_m$$

$$H_1 = \frac{J_2 s^2}{4} \sum_m \left(\mathbf{t}_m^\dagger \cdot \mathbf{t}_{m+1} + \mathbf{t}_{m+1}^\dagger \cdot \mathbf{t}_m + \mathbf{t}_m^\dagger \cdot \mathbf{t}_{m+1}^\dagger + \mathbf{t}_{m+1} \cdot \mathbf{t}_m \right)$$

The constraint

Each rung must be either singlet or triplet $\Rightarrow$ the Bosons have to obey the constraint for each rung *m*

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

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We had assumed that the singlets are condensed into the state with momentum $k = 0 \Rightarrow$ the singlet operators $s_m^\dagger$ and s_m can be replaced by a real number s

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$$N_r\, s^2 + \sum_m \mathbf{t}_m^\dagger \cdot \mathbf{t}_m = N_r$$

Fourier transformation gives

$$\sum_k \mathbf{t}_k^\dagger \cdot \mathbf{t}_k - N_r(1 - s^2) = 0$$

Spin ladders

The Hamiltonian is

$$H \quad = \quad J_1 \sum_m \mathbf{t}_m^\dagger \cdot \mathbf{t}_m + \frac{J_2 s^2}{2} \sum_m \left[\left(\mathbf{t}_{m+1}^\dagger \cdot \mathbf{t}_m + H.c \right) + \left(\mathbf{t}_m^\dagger \cdot \mathbf{t}_{m+1}^\dagger + H.c \right) \right]$$

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- The constraint was

$$\sum_k \mathbf{t}_k^\dagger \cdot \mathbf{t}_k - N_r(1 - s^2) = 0$$

- We do a Fourier transform and add the constraint with Lagrange multiplier $-\mu$

$$H = \sum_k \epsilon_k \, \mathbf{t}_k^\dagger \cdot \mathbf{t}_k + \frac{1}{2} \sum_k \Delta_k \left(\mathbf{t}_k^\dagger \cdot \mathbf{t}_{-k}^\dagger + H.c \right) + \mu N_r (1 - s^2)$$

$$\epsilon_k = J_1 + J_2 s^2 \cos(k) - \mu \qquad \Delta_k = J_2 s^2 \cos(k)$$

Spin ladders

$$H = \sum_k \epsilon_k \, \mathbf{t}_k^\dagger \cdot \mathbf{t}_k + \frac{1}{2} \sum_k \Delta_k \left(\mathbf{t}_k^\dagger \cdot \mathbf{t}_{-k}^\dagger + H.c \right) + \mu N_r (1 - s^2)$$

$$\epsilon_k = J_1 - \mu + J_2 s^2 \cos(k) \qquad \Delta_k = J_2 s^2 \cos(k)$$

We again use Bosonic Bogoliubov transformation to diagonalize H

$$\tau_k^\dagger = u_k \, \mathbf{t}_k^\dagger + v_k \, \mathbf{t}_{-k}$$

$$\tau_{-k} = v_k \, \mathbf{t}_k^\dagger + u_k \, \mathbf{t}_{-k}$$

Demanding again $[\tau_{k,\nu}, \tau_{k,\nu}^\dagger] = 1$ and $[H, \tau_{k,\nu}^\dagger] = \omega_k \tau_{k,\nu}^\dagger$ gives the triplet dispersion

$$\omega_k = \sqrt{\epsilon_k^2 - \Delta_k^2}$$

Spin ladders

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We had

$$\omega_k = \sqrt{\epsilon_k^2 - \Delta_k^2}$$

$$\epsilon_k = J_1 - \mu + J_2 s^2 \cos(k) \qquad \Delta_k = J_2 s^2 \cos(k)$$

- This involves the unknown singlet condensation amplitude s and the unknown Lagrange multiplier μ
- These can be determined by minimizing the Helmholtz Free Energy - which is the ground state energy for $T = 0$
- This can be found in my notes - and also the mean-field treatment of the quartic term

Spin ladders

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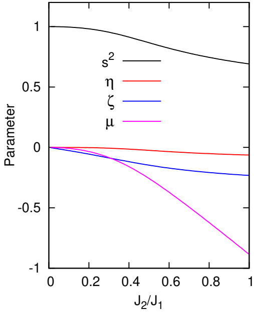
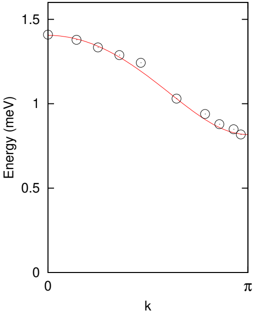
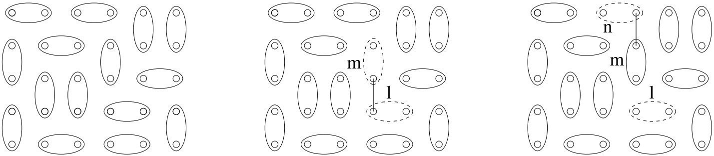




Neutron scattering on $(C_5D_{12}N)_2CuBr_4$
A.T. Savici *et al.*
PRB **80**, 094411 (2009)

Compared to theory for
$J_1 = 1.09\text{meV}$
$J_2 = 0.30\text{meV}$

Planar System



- In the treatment of ladders we saw that the excitations of the ‘singlet soup’ can be described a propagating triplets

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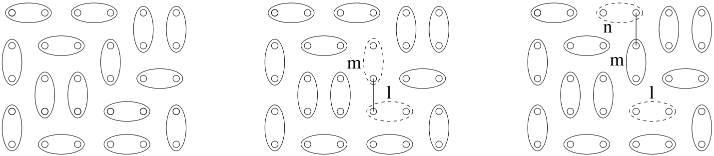

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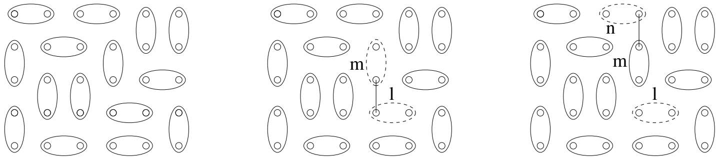

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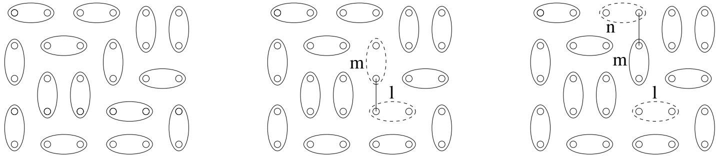

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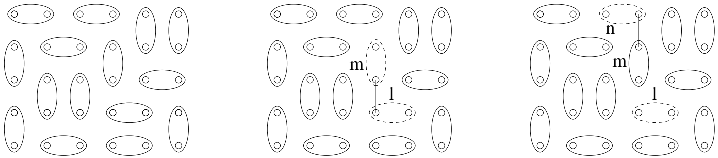

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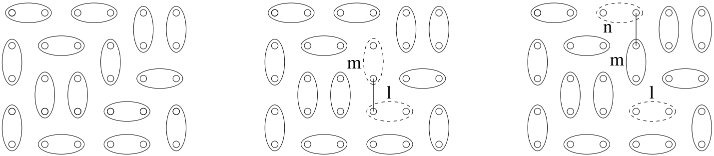
- However, the representation of the Heisenberg exchange in terms of singlets and triplets is exact for any dimer covering
- Therefore any dimer covering should give the same results
- Therefore we might come up with the idea to average the dimer Hamiltonian over all possible coverings

Planar System



- We want to average the dimer Hamiltonian over all dimer coverings
- This means we put a 'dimer' on any of the $2N$ bonds of the lattice
- The Hamitonian for two bonds m and n connected by the exchange term is

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

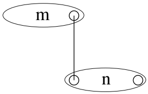
- $h_{m,n}$ is the full singlet-triplet Hamiltonian
- $N_{m,n}$: Number of dimer coverings which contain the bonds n and m
- N_d: Total number of dimer coverings

Planar System

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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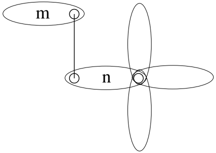

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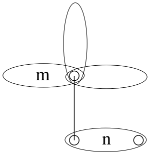

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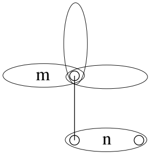

This gives $\zeta \approx \frac{1}{12}$

Planar System

The Heisenberg exchange was (i belongs to bond m, j belongs to bond n)

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

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

What we learned from the spin ladder:

- The singlet operators $s_m^\dagger$, s_m where replaced by the condensation amplitude s
- The quartic terms did not give an important correction - we may discard them
- The energy of the triplet was changed $J_1 \rightarrow J_1 - \mu$ with μ large and negative
- The approximate Hamiltonian is

Planar System

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

Planar System

In this way we obtain the final triplet Hamiltonian

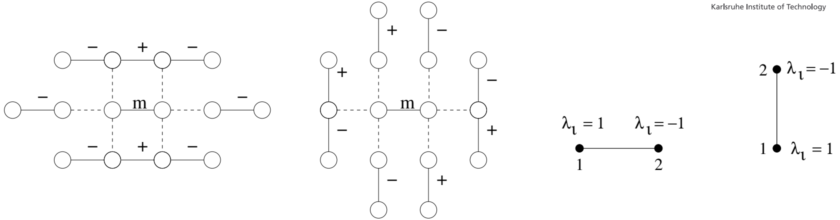
$$H = J_{eff} \sum_{m} \mathbf{t}_m^\dagger \cdot \mathbf{t}_m^\dagger + \frac{\zeta s^2}{4} \sum_{m \cap n = 0} \sum_{\substack{i \in m \\ j \in n}} J_{i,j}\, \lambda_i \lambda_j \left(\mathbf{t}_m^\dagger \cdot \mathbf{t}_n^\dagger + \mathbf{t}_n \cdot \mathbf{t}_m + \mathbf{t}_m^\dagger \cdot \mathbf{t}_n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

- Sum over $m \cap n = 0$ runs over all nonintersecting pairs of bonds in the averaged system
- $J_{i,j} = J$ 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
- If bond m connects the sites i and j we define the 'position of the bond' as

$$\mathbf{R}_m = (\mathbf{R}_i + \mathbf{R}_j)/2$$

- We have two species of bonds: x- and y-direction - and give the Fourier transform an additional index: $\mathbf{t}_{\mathbf{k},\mu}^\dagger$ with $\mu \in \{x, y\}$

Planar System



Geometry of dimers and presence of λ's gives unusual tight-binding harmonics

$$H = \sum_{\mathbf{k}} \sum_{\mu,\mu' \in \{x,y\}} \left(\mathbf{t}^{\dagger}_{\mathbf{k},\mu} \left(J_{eff}\delta_{\mu\mu'} + \epsilon_{\mu,\mu'}(\mathbf{k}) \right) \mathbf{t}_{\mathbf{k},\mu'} + \frac{1}{2} \left(\mathbf{t}^{\dagger}_{\mathbf{k},\mu}\, \epsilon_{\mu,\mu'}(\mathbf{k})\, \mathbf{t}^{\dagger}_{-\mathbf{k},\mu'} + H.c. \right) \right)$$

$$\epsilon_{x,x}(\mathbf{k}) = \zeta s^2 J \left(\cos(k_y) - \frac{1}{2}\cos(2k_x) - \cos(k_x)\cos(k_y) \right),$$

$$\epsilon_{x,y}(\mathbf{k}) = \zeta s^2 J \left(\sin(\frac{3k_x}{2})\sin(\frac{k_y}{2}) + \sin(\frac{k_x}{2})\sin(\frac{3k_y}{2}) \right),$$

Planar System

Surprisingly after doing the Bogoliubov transform we get a rather simple expression for the magnon dispersion

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

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

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

- We should now do 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 ζs^2 to reproduce two characteristic energies: bandwidth $2J$ and spin gap Δ_s

Planar System

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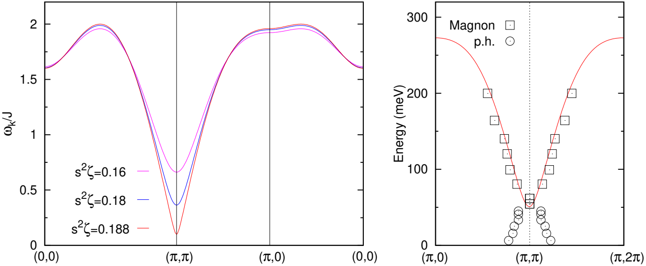

Left: Triplet dispersion with $J_{eff} = 1.7\,J$ - for ladders at $J_2 = J_1$ we had $J_{eff} = 1.8\,J$
We also recall $\zeta \approx \frac{1}{12} = 0.125$ and $s^2 = 0.8$ for ladders at $J_2 = J_1$

Right: Triplet dispersion for $J_{eff} = 1.7\,J$, $s^2\zeta = 0.16$ and $J = 140$meV compared to the 'hourglass dispersion' in $La_{1.875}Ba_{0.125}CuO_4$

Doped Holes

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

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

Doped Holes

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

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- They have spin $\pm\frac{1}{2}$ - 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

Doped Holes

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')

Similarly as for the spin operator $\mathbf{S}_i$ we can find the representation of the $\mathbf{c}_j^\dagger$-spinor

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

- The factors of $i\tau_y$ are necessary to match the transformation properties
- s and $\mathbf{t}$ are the singlet and triplet operators
- 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

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

- 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 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 details are given in my notes - we find a surprisingly simple expressions for the lowest hole-band:

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

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

Doped Holes

To determine the Fermi surface we must know how to count electrons

A singlet or triplet contain two electrons, the f-Fermions one

For a fixed dimer covering the total number of electrons is

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

Dividing by N we find the density of electrons/site

$$n_e = 1 - \frac{1}{N} \sum_{m,\sigma} \left(f_{m,+,\sigma}^\dagger f_{m,+,\sigma} + f_{m,-,\sigma}^\dagger f_{m,-,\sigma} \right)$$

Doped Holes

But: $n_e = 1 - p$ where p is the density of doped holes

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

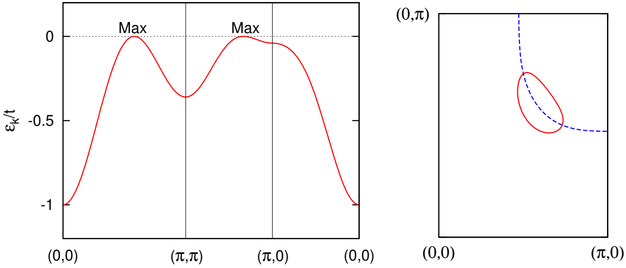
- The doped holes correspond to spin-$\frac{1}{2}$ Fermions
- The area of the Fermi surface is proportional to the density of holes
- When approaching the Mott insulator - $n_e = 1$ - the area of the Fermi surface shrinks to zero
- This is completely different from the band picture where $n_e = 1$ corresponds to a half-filled band
- We use the above expression also after the averaging procedure

Doped Holes

We found the lowest band for the Fermions

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

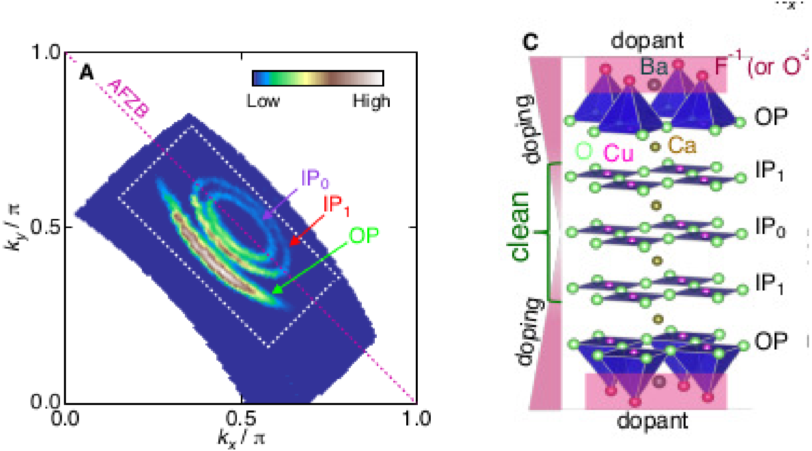
Here are results for $s^2\zeta = 0.16$



With addional hopping terms between $(1,1)$ and $(2,0)$-like neighbors the Fermi surface takes the form of a hole pocket - here $t' = -0.2t$, $t'' = 0.1t$ and the hole concentration $p = 1 - n_e = 0.1$.

Doped Holes

$Ba_2Ca_4Cu_5O_{10}(F,O)_2$ Fermi surface of $Ba_2Ca_4Cu_5O_{10}(F,O)_2$ seen in ARPES
Kunisada *et al.*, Science **369**, 833 (2020).



Summary

- For low hole concentration most electrons ‘jammed’ and retain only their spin degrees of freedom
- The mobile carriers are the doped holes
- Accordingly the system has a branch of triplet or $S = 1$ excitations and a Fermi surface with a volume proportional to the concentration p of doped holes
- This is what experiments on copper oxide superconductors have been pretty much converging to
- However, this state will not persist to higher doping
- For example, at a concentration of $p = 0.25$ each electron will find an unoccupied site on one of its 4 neighbors
- At a certain p a phase transition must occur to a state with a renormalized free-electron band and Fermi surface
- This is indeed what is see experimentally

Summary

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Phase diagram of copper-oxide superconductors