The Two-Dimensional Hubbard Model

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The Hubbard model

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

\[
H = \sum_{i,j} \sum_{\sigma} t_{i,j} \, c_{i,\sigma}^\dagger c_{j,\sigma} + U \sum_i \, n_{i,\uparrow} \, n_{i,\downarrow}
\]

\[
= \sum_{k,\sigma} \epsilon_k \, c_{k,\sigma}^\dagger c_{k,\sigma} + U \sum_i \, n_{i,\uparrow} \, n_{i,\downarrow}
\]

\[
\epsilon_k = \frac{1}{N} \sum_{i,j} e^{i k \cdot (R_i - R_j)}
\]

\[
U!
\]
\[ H = \sum_{i,j} \sum_{\sigma} t_{i,j} \sigma \cdot c_{i,\sigma}^\dagger c_{j,\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow} \]

\[ = \sum_{k,\sigma} \epsilon_k \sigma \cdot c_{k,\sigma}^\dagger c_{k,\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow} \]

\[ \epsilon_k = \frac{1}{N} \sum_{i,j} e^{ik \cdot (R_i - R_j)} \]

A very important additional parameter in this model is the density of electrons. We call \( N \) the number of sites, \( N_e = N_{\uparrow} + N_{\downarrow} \) the number of electrons - densities are denoted by \( n \): \( n_{\uparrow} = N_{\uparrow}/N \). For cuprate superconductors the important range of densities is \( 1 \geq n_e \geq 0.7 \) and \( U/t \approx 10 \). \( n_e = 1 \) means \( n_{\uparrow} = n_{\downarrow} = \frac{1}{2} \) - i.e. a metal with a half-filled band for noninteracting electrons. In contrast to this the cuprates are insulators for \( n_e = 1 \) - i.e. Mott insulators.
The Hubbard-I approximation

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

$$n_{\text{deg}} = \binom{N}{N/2}$$

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

\[ H = \sum_{i,j} \sum_\sigma \frac{t_{i,j}}{2} \left( d_{i,\sigma}^\dagger h_{j,\sim\sigma}^\dagger + H.c. \right) + \sum_{i,j} \sum_\sigma \frac{t_{i,j}}{2} \left( d_{i,\sigma}^\dagger d_{j,\sigma} - h_{i,\sim\sigma}^\dagger h_{j,\sim\sigma} \right) + U \sum_{i,\sigma} d_{i,\sigma}^\dagger d_{i,\sigma} \]
Fourier transformation gives

\[ H = \sum_{k,\sigma} \left( \left( \frac{\epsilon_k}{2} + U \right) d^\dagger_{k,\sigma} d_{k,\sigma} - \frac{\epsilon_k}{2} h^\dagger_{k,\sigma} h_{k,\sigma} \right) + \sum_{k,\sigma} \frac{\epsilon_k}{2} \left( d^\dagger_{k,\sigma} h^\dagger_{-k,-\sigma} + H.c. \right) \]

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

\[ \gamma_{-,k,\sigma} = u_k d_{k,\sigma} + v_k h^\dagger_{-k,-\sigma} \]
\[ \gamma_{+,k,\sigma} = -v_k d_{k,\sigma} + u_k h^\dagger_{-k,-\sigma} \]  \hspace{1cm} (1)

Demanding...

\[ [H, \gamma^\dagger_{\alpha,k,\sigma}] = E_k \gamma^\dagger_{\alpha,k,\sigma} \]

... leads to the eigenvalue problem

\[ \begin{pmatrix} \frac{\epsilon_k}{2} & \frac{\epsilon_k}{2} \\ \frac{\epsilon_k}{2} + U & \frac{\epsilon_k}{2} \end{pmatrix} \begin{pmatrix} u_k \\ v_k \end{pmatrix} = E_k \begin{pmatrix} u_k \\ v_k \end{pmatrix} \]
\[
\begin{pmatrix}
\frac{\epsilon_k}{2}, & \frac{\epsilon_k}{2} \\
\frac{\epsilon_k}{2}, & \frac{\epsilon_k}{2} + U
\end{pmatrix}
\begin{pmatrix}
u_k \\
v_k
\end{pmatrix}
= E_k
\begin{pmatrix}
u_k \\
v_k
\end{pmatrix}
\]

So

\[
E_{k,\pm} = \frac{1}{2} \left( \epsilon_k + U \pm \sqrt{\epsilon_k^2 + U^2} \right) \xrightarrow{U/t \to \infty} \begin{cases}
\frac{\epsilon_k}{2} + U \\
\frac{\epsilon_k}{2}
\end{cases}
\]

Example: \( U/t = 10 \)

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

Comparison with Hartree-approximation:

\( E_k = \frac{U}{2} + \epsilon_k \)
Rigorous Derivation: Equation of motion method

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

\[ c_{i,\uparrow} = c_{i,\uparrow} n_{i,\downarrow} + c_{i,\uparrow}(1 - n_{i,\downarrow}) = \hat{d}_{i,\uparrow} + \hat{c}_{i,\uparrow} \]
Rigorous Derivation: Equation of motion method

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

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

Accordingly these operators obey

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

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

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

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

\[ i \partial_t G_{\alpha,\beta}(\vec{k}, t) = \delta(t) \langle \{ \beta_{\vec{k},\sigma}^{\dagger}, \alpha_{\vec{k},\sigma} \} \rangle - i \langle T [\alpha_{\vec{k},\sigma}, H](t) \beta_{\vec{k},\sigma}^{\dagger} \rangle. \]
Consider the hopping term between the sites $i$ and $j$: 

$$ T_{i,j} = t_{i,j} \sum_\sigma \left( c_{i,\sigma}^\dagger c_{j,\sigma} + c_{j,\sigma}^\dagger c_{i,\uparrow} \right) $$ 

with 

$$ [c_{i,\sigma}, T_{i,j}] = t_{i,j} c_{j,\sigma} $$

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

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

$$ [\hat{c}_{i,\uparrow}, T_{i,j}] = [c_{i,\uparrow}, c_{i,\downarrow}, c_{i,\downarrow}^\dagger, T_{i,j}] $$

$$ = c_{i,\uparrow} c_{i,\downarrow} [c_{i,\downarrow}^\dagger, T_{i,j}] + c_{i,\uparrow} [c_{i,\downarrow}, T_{i,j}] c_{i,\downarrow}^\dagger + [c_{i,\uparrow}, T_{i,j}] c_{i,\downarrow} c_{i,\downarrow}^\dagger $$

$$ = t_{i,j}(-c_{i,\uparrow} c_{i,\downarrow} c_{j,\downarrow}^\dagger + c_{i,\uparrow} c_{j,\downarrow} c_{i,\downarrow}^\dagger + c_{j,\uparrow} c_{i,\downarrow} c_{i,\downarrow}^\dagger) $$

$$ = t_{i,j}(-c_{i,\uparrow} c_{i,\downarrow} c_{j,\downarrow}^\dagger + c_{i,\downarrow} c_{i,\uparrow} c_{j,\downarrow} + c_{j,\uparrow} (1 - n_{i,\downarrow})) $$

$$ = t_{i,j}(-c_{i,\uparrow} c_{i,\downarrow} c_{j,\downarrow}^\dagger + S_i^- c_{j,\downarrow} + c_{j,\uparrow} (1 - n_{i,\downarrow})) $$

$$ = t_{i,j}(-c_{i,\uparrow} c_{i,\downarrow} c_{j,\downarrow}^\dagger + S_i^- c_{j,\downarrow} + S_i^z c_{j,\uparrow} (1 - (\frac{n_i}{2} - S_i^z))) $$

$$ = t_{i,j}(-c_{i,\uparrow} c_{i,\downarrow} c_{j,\downarrow}^\dagger + (S_i^- c_{j,\downarrow} + S_i^z c_{j,\uparrow}) + c_{j,\uparrow} ((1 - \frac{\langle n_i \rangle}{2}) - (\frac{n_i}{2} - \frac{\langle n_i \rangle}{2})) $$
Collecting terms and writing $\langle n_i \rangle = n_e$ we find

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

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

The various terms describe

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

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

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

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

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

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

$$[\hat{d}_{i,\uparrow}, H_t] = \sum_j t_{ij} \frac{n_e}{2} c_{j,\uparrow} = \frac{n_e}{2} \sum_j t_{ij} \left(\hat{c}_{j,\uparrow} + \hat{d}_{j,\uparrow}\right)$$
Spatial Fourier transformation and adding the commutator with $H_U$ gives

$$[\hat{c}_{k,\uparrow}, H] = \left(1 - \frac{n_e}{2}\right) c_{k,\uparrow} (\hat{c}_{k,\uparrow} + \hat{d}_{k,\uparrow})$$

$$[\hat{d}_{k,\uparrow}, H] = \frac{n_e}{2} c_{k,\uparrow} (\hat{c}_{k,\uparrow} + \hat{d}_{k,\uparrow}) + U \hat{d}_{k,\uparrow}$$

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

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

$$\{\hat{d}^\dagger_{i,\sigma}, \hat{d}_{i,\sigma}\} = n_{i-\sigma}$$

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

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

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

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

\[
\begin{pmatrix}
\omega - \left(1 - \frac{n_e}{2}\right) \epsilon_k, \\
-\frac{n_e}{2} \epsilon_k, \\
\omega - \frac{n_e}{2} \epsilon_k - U
\end{pmatrix}
\begin{pmatrix}
G_{\hat{c},\hat{c}}, \\
G_{\hat{c},\hat{d}}, \\
G_{\hat{d},\hat{c}}, \\
G_{\hat{d},\hat{d}}
\end{pmatrix} =
\begin{pmatrix}
1 - \frac{n_e}{2}, \\
0, \\
0, \\
\frac{n_e}{2}
\end{pmatrix}
\]

Now we can use ....

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

... to solve for the \(2 \times 2\) matrix \(G(k, \omega)\)

Since \(c_{k,\sigma} = \hat{c}_{k,\sigma} + \hat{d}_{k,\sigma}\) the electron Green’s function

\[
G(k, t) = -i \langle T c_{k,\sigma}(t) c_{k,\sigma}^\dagger \rangle,
\]

can be obtained as \(G = G_{\hat{c},\hat{c}} + G_{\hat{c},\hat{d}} + G_{\hat{d},\hat{c}} + G_{\hat{d},\hat{d}}\)
After some algebra this can be brought to the familiar-looking form...

\[ G(k, \omega) = \frac{1}{\omega - \epsilon_k - \Sigma(\omega)} \]

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

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

This is the sum of the Hartree-Fock potential and a term with a single pole
Relation to the heuristic derivation: set $n_e = 1$

$$\left( \begin{array}{c}
i\partial_t - (1 - \frac{n_e}{2}) \epsilon_k, \\
-\frac{n_e}{2} \epsilon_k, \\
i\partial_t - \frac{n_e}{2} \epsilon_k - U\end{array} \right) \left( \begin{array}{cc} G_{\hat{c},\hat{c}} & G_{\hat{c},\hat{d}} \\
G_{\hat{d},\hat{c}} & G_{\hat{d},\hat{d}} \end{array} \right) = \delta(t) \left( \begin{array}{cc} 1 - \frac{n_e}{2} & 0 \\
0 & \frac{n_e}{2} \end{array} \right)$$
Relation to the heuristic derivation: set $n_e = 1$

$$
\left(
\begin{array}{c}
    i \partial_t - (1 - \frac{n_e}{2}) \epsilon_k , \\
    -\frac{n_e}{2} \epsilon_k ,
\end{array}
\right) \left(
\begin{array}{cc}
    G_{\hat{c},\hat{c}} & G_{\hat{c},\hat{d}} \\
    G_{\hat{d},\hat{c}} & G_{\hat{d},\hat{d}}
\end{array}
\right) = \delta(t) \left(
\begin{array}{c}
    1 - \frac{n_e}{2} , \\
    0
\end{array}
\right)$$
Relation to the heuristic derivation: set $n_e = 1$

\[
\left( i\partial_t - \frac{1}{2} \epsilon_k , -\frac{1}{2} \epsilon_k \right) \left( \begin{array}{cc} G_{\hat{c},\hat{c}} & G_{\hat{c},\hat{d}} \\ G_{\hat{d},\hat{c}} & G_{\hat{d},\hat{d}} \end{array} \right) = \delta(t) \left( \begin{array}{c} \frac{1}{2} \\ 0 \end{array} \right)
\]

Now introduce

\[
d_{i,\sigma}^\dagger = \sqrt{2} \hat{d}_{i,\sigma}^\dagger \\
h_{i,-\sigma}^\dagger = \sqrt{2} \hat{c}_{i,\sigma}
\]

\[
\left[ i\partial_t - \left( \frac{1}{2} \epsilon_k , \frac{1}{2} \epsilon_k \right) \right] \left( \begin{array}{cc} -i\langle T h_{-k,\downarrow}(t) h_{-k,\downarrow} \rangle & -i\langle T h_{-k,\downarrow}(t) d_{k,\uparrow}^\dagger \rangle \\ -i\langle T d_{k,\uparrow}(t) h_{-k,\downarrow} \rangle & -i\langle T d_{k,\uparrow}(t) d_{k,\uparrow}^\dagger \rangle \end{array} \right) = \delta(t)
\]

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

\[
H = \sum_{k,\sigma} \left( \frac{\epsilon_k}{2} + U \right) d_{k,\sigma}^\dagger d_{k,\sigma} - \frac{\epsilon_k}{2} h_{k,\sigma}^\dagger h_{k,\sigma} + \sum_{k,\sigma} \frac{\epsilon_k}{2} \left( d_{k,\sigma}^\dagger h_{-k,-\sigma}^\dagger + H.c. \right)
\]
After fixing the Fermi energy in the usual way we obtain the spectral function

\[ \Gamma(X) \]

Note the transfer of spectral weight upon decreasing electron density

(Experimental data on \( \text{La}_{2-x}\text{Sr}_x\text{CuO}_4 \) by C.T. Chen et al., Phys. Rev. Lett. 66, 104 (1991))
For small doping the Fermi surface is a small pocket around \((\pi, \pi)\) - the Fermi surface volume depends on electron density in a strange nonlinear way - this is a well-known deficiency of the Hubbard-I approximation.
Comparison to $A(k, \omega)$ obtained by QMC on an $8 \times 8$ cluster, $U/t = 8$, $n_e = \frac{1}{2}$.

QMC at $k_B T = t$ - Fermi surface volume
Rough estimate for fractional Fermi surface volume

\[ V_{Fermi} = \frac{1}{64} \sum_{k} n_k, \]

\begin{figure}
\centering
\includegraphics[width=\textwidth]{image.png}
\end{figure}
Summary: the Hubbard-I approximation

- Basic step: introduce half-filled state as ‘vacuum’
- Charge fluctuations are interpreted as hole-like and double occupancy-like ‘particles’
- The particles have energies 0 and $U \Rightarrow$ two Hubbard-bands
- For less than half-filling the lower Hubbard band is ‘hole doped’
- Fermi surface is a small hole pocket at the maximum of the lower Hubbard band (usually $(\pi, \pi)$)
- Fermi surface volume $\to 0$ as $n_e \to 1$
- Nonlinear dependence of Fermi surface volume on electron density
- Comparison with QMC: soso....
The Gutzwiller wave function

Basic idea: With increasing $U/t$ the probability to find doubly occupied sites will decrease.

This may be described by the following variational wave function

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

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

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

$$
\begin{align*}
(1 - \lambda n_{\uparrow} n_{\downarrow}) |0\rangle &= |0\rangle \\
(1 - \lambda n_{\uparrow} n_{\downarrow}) |\uparrow\rangle &= |\uparrow\rangle \\
(1 - \lambda n_{\uparrow} n_{\downarrow}) |\downarrow\rangle &= |\downarrow\rangle \\
(1 - \lambda n_{\uparrow} n_{\downarrow}) |\uparrow\downarrow\rangle &= (1 - \lambda) |\uparrow\downarrow\rangle
\end{align*}
$$

A state with $N_d$ double occupancies gets a factor of $(1 - \lambda)^{N_d} \ll 1$
Rewriting the Fermi sea $|FS\rangle$

We use (spin index suppressed!)

$$c_k^\dagger = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} e^{ik \cdot R_j} c_j^\dagger$$

Then

$$\prod_{j=1}^{M} c_{k_j}^\dagger |0\rangle = \frac{1}{\sqrt{N}^M} \sum_{i_1,i_2,i_3,\ldots,i_M} \exp \left( i \sum_{j=1}^{M} k_j \cdot R_{i_j} \right) c_{i_1}^\dagger c_{i_2}^\dagger \ldots c_{i_M}^\dagger |0\rangle$$

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

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

$$\prod_{j=1}^{M} c_{k_j}^\dagger |0\rangle = \frac{1}{\sqrt{N}^M} \sum_{i_1>i_2>i_3 \ldots >i_M} \sum_{\sigma} \exp \left( i \sum_{j=1}^{M} k_j \cdot R_{i_{\sigma(j)}} \right) c_{i_{\sigma(1)}}^\dagger c_{i_{\sigma(2)}}^\dagger \ldots c_{i_{\sigma(M)}}^\dagger |0\rangle$$
We had
\[ \prod_{j=1}^{M} c_{k_j}^\dagger |0\rangle = \frac{1}{\sqrt{N}} \sum_{i_1 > i_2 > i_3 \ldots > i_M} \sum_{\sigma} \exp \left( i \sum_{j=1}^{M} k_j \cdot R_{i_{\sigma(j)}} \right) c_{i_{\sigma(1)}}^\dagger c_{i_{\sigma(2)}}^\dagger \ldots c_{i_{\sigma(M)}}^\dagger |0\rangle \]

The product of creation operators can be brought back to the original ordered sequence
\[ c_{i_{\sigma(1)}}^\dagger c_{i_{\sigma(2)}}^\dagger \ldots c_{i_{\sigma(M)}}^\dagger |0\rangle = (-1)^{\sigma'} c_{i_1}^\dagger c_{i_2}^\dagger \ldots c_{i_M}^\dagger |0\rangle \]

Since obviously \( \sigma' = \sigma^{-1} \) we have \( (-1)^{\sigma'} = (-1)^\sigma \) we finally have
\[ \prod_{j=1}^{M} c_{k_j}^\dagger |0\rangle = \frac{1}{\sqrt{N}} \sum_{i_1 > i_2 > i_3 \ldots > i_M} \sum_{\sigma} (-1)^\sigma \exp \left( i \sum_{j=1}^{M} k_j \cdot R_{i_{\sigma(j)}} \right) c_{i_1}^\dagger c_{i_2}^\dagger c_{i_M}^\dagger |0\rangle \]
\[ = \frac{1}{\sqrt{N}} \sum_{i_1 > i_2 > i_3 \ldots > i_M} D(k_1, k_2, \ldots, k_M | i_1, i_2, \ldots, i_M) c_{i_1}^\dagger c_{i_2}^\dagger c_{i_M}^\dagger |0\rangle \]
Assuming this procedure carried out for both spin directions, the Fermi sea $|FS\rangle$ therefore may be thought of as the superposition of all real space configurations

$$D(k_1, \ldots, k_{N\uparrow}|i_1, \ldots i_{N\uparrow}) \, D(k'_{1\downarrow}, \ldots, k'_{N\downarrow}|j_1, \ldots j_{N\downarrow}) \, c_{i_1,\uparrow}^\dagger \cdots c_{i_{N\uparrow},\uparrow}^\dagger \, c_{j_{1\downarrow}}^\dagger \cdots c_{j_{N\downarrow},\downarrow}^\dagger \, |0\rangle$$

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

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

Because then each real-space configuration of electrons is included only once and all real space configurations are mutually orthogonal.
The Gutzwiller wave function can be decomposed into components with fixed number of double occupancies

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

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

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

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

Put another way: Which number of double occupancies is the most probable one?
Remember: \( |\Phi(N_d)\rangle \) is the sum over all ordered \( N^\uparrow \)-tuples \( i_1, i_2, \ldots i_{N^\uparrow} \) and \( N^\downarrow \)-tuples \( j_1, j_2, \ldots j_{N^\downarrow} \) of

\[
D(k_1, \ldots, k_{N^\uparrow} | i_1, \ldots i_{N^\uparrow}) \ D(k'_1, \ldots, k'_{N^\downarrow} | j_1, \ldots j_{N^\downarrow}) \ c^\dagger_{i_1,\uparrow} \cdots c^\dagger_{i_{N^\uparrow},\uparrow} \ c^\dagger_{j_1,\downarrow} \cdots c^\dagger_{j_{N^\downarrow},\downarrow} \ |0\rangle
\]
such that \( \{i_1, \ldots i_{N^\uparrow}\} \cap \{j_1, \ldots j_{N^\downarrow}\} \) comprises \( N_d \) sites - additional prefactor: \((1 - \lambda)^{N_d} \frac{1}{\sqrt{N^\uparrow + N^\downarrow}}\)

Since any two configurations are orthogonal we only need \( D^*(k_j | i_j) \ D(k_j | i_j) \)

\[
D(k_1, k_2, \ldots, k_M | i_1, i_2, \ldots i_M) = \sum_\sigma (-1)^\sigma \exp \left( i \sum_{j=1}^M k_j \cdot R_{i_\sigma(j)} \right)
\]

\[
D^*(k_j | i_j) \ D(k_j | i_j) = \sum_{\sigma, \sigma'} (-1)^\sigma (-1)^{\sigma'} \exp \left( i \sum_{j=1}^M k_j \cdot (R_{i_\sigma(j)} - R_{i_{\sigma'}(j)}) \right)
\]

\[
= \sum_\sigma 1 + \sum_{\sigma \neq \sigma'} (-1)^\sigma (-1)^{\sigma'} \exp \left( i \sum_{j=1}^M k_j \cdot (R_{i_\sigma(j)} - R_{i_{\sigma'}(j)}) \right)
\]

\[
= M!
\]
We want to calculate $\langle \Phi(N_d) | \Phi(N_d) \rangle$

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

$$D(k_1, \ldots, k_{N_{\uparrow}} | i_1, \ldots i_{N_{\uparrow}}) D(k'_{\downarrow}, \ldots, k'_{N_{\downarrow}} | j_1, \ldots j_{N_{\downarrow}}) c_{i_1, \uparrow}^\dagger \ldots c_{i_{N_{\uparrow}}, \uparrow}^\dagger c_{j_1, \downarrow}^\dagger \ldots c_{j_{N_{\downarrow}}, \downarrow}^\dagger |0\rangle$$

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

We have just seen that

$$D^\ast(k_j | i_j) D(k_j | i_j) = M!$$

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

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

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

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

- \( N_d \) sites with double occupancy
- \( N_{\uparrow} - N_d \) sites with \( \uparrow \)-electron only
- \( N_{\downarrow} - N_d \) sites with \( \downarrow \)-electron only
- \( N - N_d - (N_{\uparrow} - N_d) - (N_{\downarrow} - N_d) = N - N_{\uparrow} - N_{\downarrow} + N_d \) empty sites

The answer then is the multinomial coefficient

\[
C(N_{\uparrow}, N_{\downarrow}, N_d) = \frac{N!}{N_d! (N_{\uparrow} - N_d)! (N_{\downarrow} - N_d)! (N - N_{\uparrow} - N_{\downarrow} + N_d)!}
\]
We briefly remember what we are currently working on....

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

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

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

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

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

\[
\log(N!) \approx N \log(N) - N
\]

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

...and differentiate with respect to \( N_d \):

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

\[
\frac{d^2}{dN_d^2} \log(W(N_d)) = - \left( \frac{1}{N_d} + \frac{1}{N^{\uparrow} - N_d} + \frac{1}{N^{\downarrow} - N_d} + \frac{1}{1 - N^{\uparrow} - N^{\downarrow} + N_d} \right)
\]
We had

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

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

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

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

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

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

\[
(1 - \lambda)^2 \frac{(n_\uparrow - n_d) (n_\downarrow - n_d)}{n_d (1 - n_\uparrow - n_\downarrow + n_d)} = 1
\]
The first equation gives us the value of \( n_d = N_d / N \) where \( \langle \Phi(N_d) | \Phi(N_d) \rangle \) is a maximum:

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

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

\[
(1 - \lambda)^2 \frac{\left(\frac{1}{2} - n_d\right)^2}{n_d^2} = 1 \rightarrow n_d = \frac{1 - \lambda}{2(2 - \lambda)}
\]

Check: \( \lambda \rightarrow 0 \) - i.e. no projection - implies \( n_d = 1/4 = n_{\uparrow} \cdot n_{\downarrow} \) - correct at half-filling!
The second equation was

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

Here \( c \) is of order unity

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

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

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

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

\( \rightarrow \) The whole Gutzwiller wave function consists exclusively of configurations with \( N_d = N \cdot n_{d,max}! \)
We saw: The whole Gutzwiller wave function consists exclusively of configurations with a fixed $N_d = N \cdot n_d$ and $n_d$ is shifted by varying $\lambda$

![Graph showing the distribution of $n_d$](image)

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

The expectation value of $H_t$ is more difficult....
Basic idea: Reducing the number of double occupancies reduces the number of ‘hopping possibilities’
Basic idea: Reducing the number of double occupancies reduces the number of ‘hopping possibilities’
The Gutzwiller Approximation

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

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

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

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

The evaluation of the $\eta_\sigma(n_\uparrow, n_\downarrow, n_d)$ then is a combinatorical problem - this is discussed very understandably by Ogawa et al. Progr. Theor. Phys. 53, 614 (1975).
Introduce 4 ‘book-keeping kets’ for every site \( i \): \(|i, 0\rangle, |i, \uparrow\rangle, |i, \downarrow\rangle\) and \(|i, \uparrow\downarrow\rangle\).

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

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

\[
\langle B_i | B_i \rangle = 1
\]

... and the wave function of the whole lattice

\[
|\Psi\rangle = \prod_i |B_i\rangle
\]

\[
\langle \Psi | \Psi \rangle = 1
\]
We had

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

$$|\Psi\rangle = \prod_i |B_i\rangle$$

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

$$\langle N\uparrow \rangle = N \frac{\alpha^2 + \beta^2}{1 + \alpha^2 + \alpha^2 + \beta^2},$$

$$\langle N_d \rangle = N \frac{\beta^2}{1 + \alpha^2 + \alpha^2 + \beta^2}.$$ 

which can be reverted to give

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

$$\beta = \sqrt{\frac{n_d}{1 - n\uparrow - n\downarrow + n_d}}.$$
Our auxiliary wave function was (remember: \( (\alpha^\uparrow, \alpha^\downarrow, \beta) \leftrightarrow (n^\uparrow, n^\downarrow, n_d) \))

\[
|B_i\rangle = \frac{|i, 0\rangle + \alpha^\uparrow|i, \uparrow\rangle + \alpha^\downarrow|i, \downarrow\rangle + \beta|i, \uparrow\downarrow\rangle}{\sqrt{1 + \alpha^2 + \alpha^2 + \beta^2}}
\]

\[
|\Psi\rangle = \prod_i |B_i\rangle
\]

\(|\Psi\rangle\) has norm 1 and as many ‘empty sites’, ‘singly occupied sites’ and ‘doubly occupied sites’ as the true Gutzwiller wave function if we adjust \( \alpha, \sigma \) and \( \beta \) correctly.

But: \(|\Psi\rangle\) does not have fixed electron number \( \Rightarrow \) in principle we should instead use

\[
|\Psi'\rangle = \mathcal{P}(N^\uparrow, N^\downarrow, N_d) |\Psi\rangle
\]

where \( \mathcal{P} \) projects onto the component of \(|\Psi\rangle\) which has precisely \( \langle N^\uparrow \rangle \) \( \uparrow \)-electrons etc.
But: It is straightforward to show that the values of $N_{\alpha}$ - with $\alpha \in \{\uparrow, \downarrow, d\}$ have a Gaussian distribution around their mean values $\bar{N}_{\alpha}$ with a width which is again $\propto N^{-1/2}$

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

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

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

(compare J. Bardeen, L. N. Cooper, and J. R. Schrieffer Phys. Rev. 106, 162 (1957))
Our auxiliary wave function was (remember: \((\alpha_\uparrow, \alpha_\downarrow, \beta) \leftrightarrow (n_\uparrow, n_\downarrow, n_d)\))

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

\[
|\Psi\rangle = \prod_i |B_i\rangle
\]

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

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

Then we estimate the number of hopping possibilities per bond as

\[
h(\uparrow, n_\uparrow, n_\downarrow, n_d) = \frac{\langle \Psi | \tilde{c}_{i, \uparrow}^\dagger \tilde{c}_{j, \uparrow} | \Psi \rangle}{\langle \Psi | \Psi \rangle} = \langle \Psi | \tilde{c}_{i, \uparrow}^\dagger \tilde{c}_{j, \uparrow} | \Psi \rangle = \langle B_i | \tilde{c}_{i, \uparrow}^\dagger | B_i \rangle \langle B_j | \tilde{c}_{j, \uparrow} | B_j \rangle
\]

\[
= |\langle B_i | \tilde{c}_{i, \uparrow} | B_i \rangle|^2 = \left( \frac{\alpha_\uparrow + \alpha_\downarrow \beta}{1 + \alpha_\uparrow^2 + \alpha_\downarrow^2 + \beta^2} \right)^2
\]
We remember:
Our auxiliary wave function was (remember: \((\alpha_{\uparrow}, \alpha_{\downarrow}, \beta) \leftrightarrow (n_{\uparrow}, n_{\downarrow}, n_d)\))

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

\[
|\Psi\rangle = \prod_i |B_i\rangle
\]

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

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

Then we estimate the number of hopping possibilities per bond as

\[
h(\uparrow, n_{\uparrow}, n_{\downarrow}, n_d) = \frac{\langle \Psi | \tilde{c}_{i, \uparrow}^\dagger \tilde{c}_{j, \uparrow} | \Psi \rangle}{\langle \Psi | \Psi \rangle} = \langle \Psi | \tilde{c}_{i, \uparrow}^\dagger \tilde{c}_{j, \uparrow} | \Psi \rangle = \langle B_i | \tilde{c}_{i, \uparrow}^\dagger | B_i \rangle \langle B_j | \tilde{c}_{j, \uparrow} | B_j \rangle
\]

\[
= |\langle B_j | \tilde{c}_{j, \uparrow} | B_j \rangle|^2 = \left( \frac{\alpha_{\uparrow} + \alpha_{\downarrow} \beta}{1 + \alpha_{\uparrow}^2 + \alpha_{\downarrow}^2 + \beta^2} \right)^2
\]
\[ h(\sigma, n_\uparrow, n_\downarrow, n_d) = \left( \frac{\alpha_\sigma + \alpha_{-\sigma} \beta}{1 + \alpha_\uparrow^2 + \alpha_\downarrow^2 + \beta^2} \right)^2 \]

But we found earlier that \( \alpha_\sigma \) and \( \beta \) can be expressed by \( n_\sigma \) and \( n_d \)....

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

.... and inserting this we find

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

The final renormalization factor then is obtained by dividing

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

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

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

and found the terms of the sum ‘infinitely sharply peaked’ around $N_d = N \cdot n_d$ with

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

This equation allows to switch from $\lambda \rightarrow n_d$ as variational parameter!
The expectation value of $H_U$ then becomes trivial

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

The expectation value of the kinetic energy was approximated as

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

where the renormalization factors $\eta_{\sigma}$ are again functions of $n_\uparrow$, $n_\downarrow$ and $n_d$

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

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

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

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

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

where \( t_0 \) is the noninteracting kinetic energy per site - which can be obtained by numerical integration

\[ t_0 = \frac{2}{N} \sum_{k} \epsilon_k \ \Theta(E_F - \epsilon_k) \]

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

\[ \eta(n_d) = 16 \ n_d \left( \frac{1}{2} - n_d \right) \]

\[ e(n_d) = 16 \ n_d \left( \frac{1}{2} - n_d \right) \ t_0 + U \ n_d \]

Then we find the optimal \( n_d \)

\[ n_d = \frac{1}{4} - \frac{U}{32|t_0|} \]
The $n_d$ which minimizes the energy was

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

This decreases linearly with $U$ and becomes zero for

$$U_c = 8|t_0|$$

This is the famous Brinkman-Rice transition

For the 2D square lattice with nearest neighbor hopping we obtain $t_0 = -1.621 \ t \rightarrow U_c = 12.969 \ t$
Quasiparticle Dispersion

The Gutzwiller wave function was

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

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

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

The ‘quasiparticle dispersion’ then can be obtained from

$$\tilde{\epsilon}_k = \frac{\langle \Phi_G | H | \Phi_G \rangle}{\langle \Phi_G | \Phi_G \rangle} - \frac{\langle \Phi_G(k) | H | \Phi_G(k) \rangle}{\langle \Phi_G(k) | \Phi_G(k) \rangle}$$
\[ |\Phi_G(k)\rangle = \prod_i (1 - \lambda' n_i \uparrow n_i \downarrow) \ c_{k \uparrow} |FS\rangle, \]

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

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

The variational procedure for \( |\Phi_G(k)\rangle \) amounts to

\[ e \to e - \frac{1}{N} \tilde{\epsilon}_k \]
\[ t_0 \to t_0 - \frac{1}{N} \epsilon_k \]
\[ n_\uparrow \to n_\uparrow - \frac{1}{N} \]
\[ n_d \to n_d + \frac{1}{N} \delta n_d \]

Inserting and expanding gives

\[ e - \frac{1}{N} \tilde{\epsilon}_k = \left( \eta(n_\sigma, n_d) - \frac{1}{N} \frac{\partial \eta}{\partial n_\uparrow} + \frac{1}{N} \frac{\partial \eta}{\partial n_d} \delta n_d \right) \left( t_0 - \frac{1}{N} \epsilon_k \right) + n_d \ U + \frac{1}{N} \delta n_d \ U \]
\[ |\Phi_G(k)\rangle = \prod_i (1 - \lambda' n_{i,\uparrow} n_{i,\downarrow}) c_{k,\uparrow} |FS\rangle, \]

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

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

The variational procedure for \( |\Phi_G(k)\rangle \) amounts to

\[
\begin{align*}
e &\rightarrow e - \frac{1}{N} \tilde{\epsilon}_k \\
t_0 &\rightarrow t_0 - \frac{1}{N} \epsilon_k \\
n_{\uparrow} &\rightarrow n_{\uparrow} - \frac{1}{N} \\
n_d &\rightarrow n_d + \frac{1}{N} \delta n_d
\end{align*}
\]

Inserting and expanding gives

\[
\tilde{\epsilon}_k = \eta(n_\sigma, n_d) \epsilon_k + t_0 \frac{1}{2} \left( \frac{\partial \eta_{\uparrow}}{\partial n_{\uparrow}} + \frac{\partial \eta_{\downarrow}}{\partial n_{\uparrow}} \right) - \delta n_d \left( \frac{\partial \eta}{\partial n_d} t_0 + U \right)
\]
We thus find that the quasiparticle dispersion is renormalized by the same factor $\eta$ as the expectation value of the kinetic energy (the constant can be compensated by a shift of $\mu$)

$$\tilde{\epsilon}_k = \eta(n_{\sigma}, n_d) \epsilon_k + t_0 \frac{1}{2} \left( \frac{\partial \eta_\uparrow}{\partial n_\uparrow} + \frac{\partial \eta_\downarrow}{\partial n_\uparrow} \right)$$

Moreover:

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

The Gutzwiller wave function describes the metal insulator transition by the vanishing of the bandwidth
Suppose we have a ratio $U/t$ such that the system is a Mott-insulator at half-filling

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

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

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

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

We consider the case of large $U/t$ where the system is a Mott-insulator at half-filling. Then we ask: how does the system behave as $n_e \to 1$ from below? Interestingly Hubbard-I approximation and Gutzwiller wave function describe two completely different scenarios.
Experimentally it seems that Hubbard-I is closer to reality....

(Data from W. J. Padilla et al., PRB 72,060511 (2005) - remember: \( n_e = 1 - x \))
The Hubbard-I and Gutzwiller approximation are highly oversimplified. We have seen in the derivation of the Hubbard-I approximation that the coupling to spin- and density-excitations - or more generally: the collective excitations of the system - is ignored. This is in fact probably the key problem to be solved.....

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

We will proceed in three steps:

Derive an effective Hamiltonian for the lower Hubbard band
Discuss the collective excitations for the antiferromagnetic phase: magnons
Discuss the effect of the coupling of the magnons to a single mobile hole
It will be seen that the modifications as compared to Hubbard-I are drastic.....
Strong coupling expansion

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

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

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

To that end we use a canonical transformation plus perturbation theory
The Hilbert space can be decomposed into ‘sectors’ with fixed number of double occupancies

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

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

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

\[ H = H_0 + H_1 \]

\[ H_0 = \sum_{i,j} \sum_{\sigma} t_{i,j} (\hat{c}_{i,\sigma} \hat{c}_{j,\sigma} + \hat{d}_{i,\sigma} \hat{d}_{j,\sigma}) + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow} \]

\[ H_1 = \sum_{i,j} \sum_{\sigma} t_{i,j} (\hat{d}_{i,\sigma} \hat{c}_{j,\sigma} + \hat{c}_{i,\sigma} \hat{d}_{j,\sigma}) \]
We consider canonical transformations of the Hilbert space

\[ |\Psi'\rangle = e^S |\Psi\rangle \]

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

Unitarity of \( e^S \) requires \( S^\dagger = -S \)

Example: for \( S = \frac{i}{\hbar} H t \) this is the transformation Schrödinger picture → Heisenberg picture
The transformation was

\[ |\Psi'\rangle = e^S |\Psi\rangle \]

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

Our goal: Find an \( S \) such that ‘connecting part’ \( H_1 \) is eliminated from \( H' \)

Insert \( \hat{O} \rightarrow H_0 + H_1 \):

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

\[ |\Psi'\rangle = e^S |\Psi\rangle \]

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

Our goal: Find some \( S \) such that ‘connecting part’ \( H_1 \) is eliminated from \( H' \)

Insert \( \hat{O} \to H_0 + H_1 \):

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

Now choose \( S \) such that

\[ H_1 + [S, H_0] = 0 \]
Then $H'$ becomes (using $[S, H_0] = -H_1$)

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

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

Obviously this makes sense only if $S$ is ‘small’ in some sense so that higher order terms can be neglected.
In our application to the Hubbard model we had (remember: \( U \gg t_{i,j} \))

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

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

The requirement on \( S \) was

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

We recall the commutator relation for the Hubbard-operators

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

and guess easily (?)

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

\[
[S, H_U] = \sum_{i,j} \sum_{\sigma} \frac{t_{i,j}}{U} \left( [\hat{d}_{i,\sigma}, H_U] \hat{c}_{j,\sigma} - \hat{c}_{i,\sigma}^\dagger [\hat{d}_{i,\sigma}, H_U] \right)
\]
In our application to the Hubbard model we had (remember: $U \gg t_{i,j}$)

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

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

The requirement on $S$ was

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

We recall the commutator relation for the Hubbard-operators

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

and guess easily (?)

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

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

\[ S = \sum_{i,j} \sum_{\sigma} t_{i,j} \frac{U}{\sigma} (\hat{d}_{i,\sigma} \hat{c}_{j,\sigma} - \hat{c}_{i,\sigma} \hat{d}_{j,\sigma}) \]

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

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

\[ \approx H_0 + \frac{1}{2} [S, H_1] \]

The lowest order correction term then becomes

\[ H'_c = \frac{1}{2} [S, H_1] = \frac{1}{2} \sum_{i,j,l,m} \sum_{\sigma,\sigma'} \frac{t_{i,j} t_{l,m}}{U} \left[ \hat{d}_{i,\sigma} \hat{c}_{j,\sigma} - \hat{c}_{i,\sigma} \hat{d}_{j,\sigma} + \hat{d}_{i,\sigma'} \hat{c}_{m,\sigma} + \hat{c}_{i,\sigma'} \hat{d}_{m,\sigma} \right] \]

\[ = -\frac{1}{2} \sum_{i,j,l} \sum_{\sigma,\sigma'} \frac{t_{i,j} t_{l,i}}{U} \hat{c}_{i,\sigma} \hat{d}_{i,\sigma'} \hat{d}_{i,\sigma} \hat{c}_{j,\sigma} - \frac{1}{2} \sum_{i,j,m} \sum_{\sigma,\sigma'} \frac{t_{i,j} t_{j,m}}{U} \hat{c}_{i,\sigma} \hat{d}_{j,\sigma} \hat{d}_{j,\sigma} \hat{c}_{m,\sigma'} \]

\[ = -\sum_{i,j,l} \sum_{\sigma,\sigma'} \frac{t_{i,l} t_{j,i}}{U} \hat{c}_{i,\sigma} \hat{d}_{l,\sigma'} \hat{d}_{l,\sigma} \hat{c}_{j,\sigma} \]
After a straightforward but lengthy calculation we find

\[
H_{sc} = \sum_{i,j} \sum_{\sigma} t_{i,j} \hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} + \sum_{i,j} J_{i,j} \left( \mathbf{S}_i \cdot \mathbf{S}_j - \frac{n_i n_j}{4} \right) - \sum_{i,j,l} \frac{t_{i,l} t_{l,j}}{U} \left( \left( \hat{c}_{i,\uparrow}^\dagger n_{i,\uparrow} \hat{c}_{j,\downarrow} - \hat{c}_{i,\uparrow}^\dagger S_{l}^{-} \hat{c}_{j,\downarrow} \right) + (\downarrow \leftrightarrow \uparrow) \right)
\]
After a straightforward but lengthy calculation we find

\[
H_{sc} = \sum_{i,j} \sum_{\sigma} t_{i,j} \hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} + \sum_{i,j} J_{i,j} \left( \left( S^z_i S^z_j + \frac{1}{2} \left( S^+_i S^-_j + S^-_i S^+_j \right) \right) - \frac{n_i n_j}{4} \right) \\
- \sum_{i,j,l} t_{i,l} t_{l,j} \frac{U}{U} \left( \left( \hat{c}_{i,\downarrow} n_{i,\uparrow} \hat{c}_{j,\downarrow} - \hat{c}_{i,\uparrow} S^-_l \hat{c}_{j,\downarrow} \right) + (\downarrow \leftrightarrow \uparrow) \right)
\]
After a straightforward but lengthy calculation we find

\[
H_{sc} = \sum_{i,j} \sum_{\sigma} t_{i,j} \hat{c}_{i,\sigma}^{\dagger} \hat{c}_{j,\sigma} + \sum_{i,j} J_{i,j} \left( \left( S_i^z S_j^z + \frac{1}{2} \left( S_i^+ S_j^- + S_i^- S_j^+ \right) \right) - \frac{n_i n_j}{4} \right) \\
- \sum_{i,j,l} t_{i,l} t_{l,j} \frac{U}{U} \left( (\hat{c}_{i,\downarrow} n_{l,\uparrow} \hat{c}_{j,\downarrow} - \hat{c}_{i,\uparrow} S_{l}^- \hat{c}_{j,\downarrow}) + (\downarrow \leftrightarrow \uparrow) \right)
\]
Spin waves

The strong coupling Hamiltonian in the sector without double occupancies was

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

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

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

\[ H_{sc} = \sum_{i,j} J_{i,j} \left( S_i \cdot S_j - \frac{n_i n_j}{4} \right) \]

Further simplifications:

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

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

\[ H_{sc} = J \sum_{\langle i,j \rangle} S_i \cdot S_j \]

\[ = J \sum_{\langle i,j \rangle} \left( S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z \right) \]

\[ = J \sum_{\langle i,j \rangle} \left( S_i^z S_j^z + \frac{1}{2} \left( S_i^+ S_j^- + S_i^- S_j^+ \right) \right) \]
The Heisenberg antiferromagnet

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

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

However, the Néel state is not an eigenstate of the full Hamiltonian because the transverse part can produce quantum fluctuations.
To deal with the quantum fluctuations we represent the inverted spins as Bosons

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

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

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

\[
= \frac{J}{2} \sum_{i \in \uparrow-SL} \sum_{j \in N(i)} \left( a_i^\dagger b_j^\dagger + b_j a_i \right)
\]
Geometry of the lattice
Hamiltonian for the Bosons

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

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

The transverse part creates/annihilates pairs of inverted spins on nearest neighbors
Each inverted spin increases the expectation value of the term $J \sum_{\langle i,j \rangle} S_i^z S_j^z$

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

$$J \sum_{\langle i,j \rangle} S_i^z S_j^z = \frac{zJ}{2} \left( \sum_{i \in \uparrow-\downarrow} a_i^\dagger a_i + \sum_{j \in \uparrow-\downarrow} b_j^\dagger b_j \right)$$
In this way we have ‘translated’ the Hamiltonian of the Heisenberg antiferromagnet into the Boson formulation

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

Fourier transformation yields

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

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

Thereby \( \mathbf{k} \) is a momentum from the antiferromagnetic Brillouin zone:
$$H_{SW} = \frac{zJ}{2} \sum_{\mathbf{k}} \left( a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + b_{\mathbf{k}}^\dagger b_{\mathbf{k}} + \gamma_{\mathbf{k}} (a_{\mathbf{k}}^\dagger b_{-\mathbf{k}}^\dagger + b_{-\mathbf{k}} a_{\mathbf{k}}) \right),$$

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

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

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

Then $H$ can be diagonalized by a Bosonic Bogoliubov transformation

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

Demanding that the magnon operators $\gamma_{a,\mathbf{k}}$ are Bosons: $[\gamma_{a,\mathbf{k}}, \gamma_{a,\mathbf{k}}^\dagger] = 1$, requires $u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2 = 1$ and demanding $[H, \gamma_{a,\mathbf{k}}^\dagger] = \omega_{\mathbf{k}} \gamma_{a,\mathbf{k}}^\dagger$ gives

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

with $\gamma_{\mathbf{k}} = \frac{1}{4} \left( 2 \cos(k_x) + 2 \cos(k_y) \right)$, $\nu_{\mathbf{k}} = \sqrt{1 - \gamma_{\mathbf{k}}^2}$.
Propagation of a magnon

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Propagation of a magnon

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Propagation of a magnon
Propagation of a magnon

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Propagation of a magnon

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Application: Dispersion and spectral weight of magnons in La$_2$CuO$_4$

We had: $\omega_k = \frac{zJ}{2} \sqrt{1 - \gamma_k^2}$

$I_k \propto (u_k \pm v_k)^2$

Inelastic neutron scattering results from R. Coldea et al., PRL 86, 5377 (2001)
Reminder: in our derivation we have simply ignored the hard-core constraint and treated the Bosons as free particles - is this justified? Using the reverse Bogoliubov transformation....

\[ a_\mathbf{k}^\dagger = u_\mathbf{k} \gamma_{a,\mathbf{k}} - v_\mathbf{k} \gamma_{b,-\mathbf{k}} \]
\[ b_{-\mathbf{k}} = -v_\mathbf{k} \gamma_{a,\mathbf{k}} + u_\mathbf{k} \gamma_{b,-\mathbf{k}} \]

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

\[ n_a = \frac{2}{N} \sum_{\mathbf{k}} \langle \text{GS}| a_{\mathbf{k}}^\dagger a_{\mathbf{k}} |\text{GS}\rangle \]
\[ = \frac{2}{N} \sum_{\mathbf{k}} \langle \text{GS}| (u_\mathbf{k} \gamma_{a,\mathbf{k}}^\dagger - v_\mathbf{k} \gamma_{b,-\mathbf{k}}) (u_\mathbf{k} \gamma_{a,\mathbf{k}} - v_\mathbf{k} \gamma_{b,-\mathbf{k}}^\dagger) |\text{GS}\rangle \]
\[ = \frac{2}{N} \sum_{\mathbf{k}} v_\mathbf{k}^2 \]

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

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

- We specialize to the case \( N_e = N - 1 \) - a single hole in the Mott insulator
- For simplicity we discard the three-site hopping terms
- In addition we assume hopping \( t_{i,j} \) and exchange \( J_{i,j} \) only between nearest neighbors
- The remaining Hamiltonian is called the t-J model
• Basic assumption: a single hole will not destroy antiferromagnetic order
• We continue to use the Néel state as a starting point of the discussion
• Assume that the electron on site $i \in \uparrow - SL$ of the Néel state has been removed

![Diagram showing spin configuration]

- The term $-t \hat{c}^\dagger_{i,\downarrow} \hat{c}_{j,\downarrow}$ can transport the hole
- But thereby an inverted spin on site $i$ is left behind
- This is a magnon as introduced in the preceding discussion
- The hole ‘radiates off’ magnons as it propagates
Collecting terms and writing $\langle n_i \rangle = n_e$ we find

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

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

The various terms describe

Coherent propagation from $i \to j$

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

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

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

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

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

$$[\hat{d}_{i,\uparrow}, H_t] = \sum_j t_{ij} \frac{n_e}{2} c_{j,\uparrow} = \frac{n_e}{2} \sum_j t_{ij} (\hat{c}_{j,\uparrow} + \hat{d}_{j,\uparrow})$$
• Basic assumption: a single hole will not destroy antiferromagnetic order
• We continue to use the Néel state as a starting point of the discussion
• Assume that the electron on site \( i \in \uparrow -SL \) of the Néel state has been removed

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\uparrow & \downarrow & \uparrow & \downarrow & \uparrow & \downarrow & \uparrow & \downarrow \\
\downarrow & \cdot & \downarrow & j & \uparrow & \downarrow & \cdot & \uparrow \\
\uparrow & \downarrow & \uparrow & \downarrow & \uparrow & \downarrow & \uparrow & \downarrow \\
\end{array}
\]

\( (a) \) \hspace{1cm} \( (b) \)

• The term \(-t \hat{c}_{i,\uparrow}^\dagger \hat{c}_{j,\uparrow}\) can transport the hole
• But thereby an inverted spin on site \( i \) is left behind
• This is a magnon as introduced in the preceding discussion

• The hole ‘radiates off’ magnons as it propagates
- We introduce Fermions $h_{a,i}^\dagger$ for $i \in \uparrow$-SL and $h_{b,j}^\dagger$ for $j \in \uparrow$-SL
- we continue to use $a_i^\dagger$ (inverted spin at site $i \in \uparrow$-SL) and $b_j^\dagger$ (inverted spin at site $j \in \downarrow$-SL)

This is described by the Hamiltonian

\[
H_{int} = t \sum_{i \in A} \sum_n \left( h_{b,i+n}^\dagger h_{a,i} + H.c. \right) + t \sum_{j \in B} \sum_n \left( h_{a,j+n}^\dagger h_{b,j} + H.c. \right).
\]
We had
\[
H_{\text{int}} = t \sum_{i \in A} \sum_n \left( h_{b,i+n}^\dagger h_{a,i} a_i^\dagger + H.c. \right) + t \sum_{j \in B} \sum_n \left( h_{a,j+n}^\dagger h_{b,j} b_j^\dagger + H.c. \right).
\]

Fourier transformation gives (with $\epsilon_k = 2t(\cos(k_x) + \cos(k_y))$)
\[
H_{\text{int}} = \sqrt{\frac{2}{N}} \sum_{k,q} \left( \left( \epsilon_{k-q} h_{b,k-q}^\dagger h_{a,k} a_q^\dagger + H.c. \right) + (a \leftrightarrow b) \right).
\]

Now we recall the Bogoliubov transformation which diagonalized the spin wave Hamiltonian
\[
\begin{align*}
\gamma_{a,k}^\dagger &= u_k a_k^\dagger + v_k b_{-k} \\
\gamma_{b,-k}^\dagger &= u_k b_{-k}^\dagger + v_k a_k.
\end{align*}
\]

Replacing $(a_k^\dagger, b_k^\dagger) \rightarrow (\gamma_{a,k}^\dagger, \gamma_{b,k}^\dagger)$ and adding the Hamiltonian for the $\gamma$'s we finally obtain
\[
H_{\text{tot}} = \sqrt{\frac{2}{N}} \sum_{k,q} \left( \left( M(k, q) h_{b,k-q}^\dagger h_{a,k} \gamma_{a,q}^\dagger + H.c. \right) + (a \leftrightarrow b) \right) + \sum_q \omega_q \left( \gamma_{a,q}^\dagger \gamma_{a,q} + \gamma_{b,q}^\dagger \gamma_{b,q} \right).
\]
Collecting everything

\[ H_{\text{tot}} = \sqrt{\frac{2}{N}} \sum_{k,q} \left( \left( M(k, q) \ h_{b,k-q}^\dagger h_{a,k} \ \gamma_{a,q}^\dagger \right) + (a \leftrightarrow b) \right) + \sum_q \omega_q \left( \gamma_{a,q}^\dagger \gamma_{a,q} + \gamma_{b,q}^\dagger \gamma_{b,q} \right) \]

- \( M(k, q) = \epsilon_{k-q} u_q - \epsilon_k v_q \)
- \( \epsilon_k = 2t \left( \cos(k_x) + \cos(k_y) \right) \)
  \[ \gamma_{a,k}^\dagger = u_k \ a_k^\dagger + v_k \ b_{-k} \]
  \[ \gamma_{b,-k}^\dagger = u_k \ b_{-k}^\dagger + v_k \ a_k \]
- \( \omega_q = \frac{zJ}{2} \sqrt{1 - \gamma_q^2} \)
- \( \gamma_k = \frac{1}{z} \sum_n e^{i k \cdot n} = \frac{1}{4} \left( 2 \cos(k_x) + 2 \cos(k_y) \right) \)
We have to use an approximation - widely used is the self-consistent Born approximation (SCBA)

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

Define time ordered Green’s functions (⟨...⟩: expectation value in the state with no hole and no magnons)

\[ G_\alpha(k, t) = -i\langle T h_{\alpha,k}(t) h_{\alpha,k}^\dagger(0) \rangle \]
\[ B_\alpha(q, t) = -i\langle T \gamma_{\alpha,q}(t) \gamma_{\alpha,q}^\dagger(0) \rangle, \]

Diagrams for the self-energy

\[ \Sigma_\alpha(k, \omega) = \frac{i}{2\pi} \frac{2}{N} \sum_q \int d\nu \left[ M^2(k, q) B_\alpha(q, \nu) G_b(k - q, \omega - \nu) + M^2(k + q, q) B_\alpha(q, \nu) G_b(k + q, \omega + \nu) \right] \]
We had

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

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

$$B^{(0)}_\alpha(q, t) = -ie^{-i\omega q t} \left( \Theta(t) \langle \gamma_{\alpha, q} \gamma_{\alpha, q}^\dagger \rangle + \Theta(-t) \langle \gamma_{\alpha, q}^\dagger \gamma_{\alpha, q} \rangle \right) = -i\Theta(t) e^{-i\omega q t},$$

with Fourier transform

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

so that

$$\Sigma_a(k, \omega) = \frac{i}{2\pi} \frac{2}{N} \sum_q \int d\nu \left[ M^2(k, q) \frac{G_b(k - q, \omega - \nu)}{\nu - \omega_q + i0^+} + M^2(k + q, q) \frac{G_b(k + q, \omega + \nu)}{\nu - \omega_q + i0^+} \right].$$
Short digression: The Hamiltonian was

$$H = \sqrt{\frac{2}{N}} \sum_{k,q} \left( \left( M(k, q) \ h_{b,k-q}^\dagger \ h_{a,k} \ \gamma_{a,q}^\dagger + H.c. \right) + (a \leftrightarrow b) \right) + \sum_q \omega_q \left( \gamma_{a,q}^\dagger \gamma_{a,q} + \gamma_{b,q}^\dagger \gamma_{b,q} \right)$$

→ The hole Green’s function is ($\alpha \in a, b$)

$$G_\alpha(q, t) = -i \left( \Theta(t) \ \langle e^{iHt} h_{\alpha,q} e^{-iHt} h_{\alpha,q}^\dagger \rangle - \Theta(-t) \ \langle h_{\alpha,q}^\dagger e^{iHt} h_{\alpha,q} e^{-iHt} \rangle \right)$$
Short digression: The Hamiltonian was

\[ H = \sqrt{\frac{2}{N}} \sum_{k,q} \left( \left( M(k, q) \, h_{b,k-q}^\dagger \, h_{a,k} \, \gamma_{a,q} + H.c. \right) + (a \leftrightarrow b) \right) + \sum_q \, \omega_q \, \left( \gamma_{a,q} \gamma_{a,q} + \gamma_{b,q} \gamma_{b,q} \right) \]

→ The hole Green’s function is \( (\alpha \in a, b) \)

\[ G_\alpha(q, t) = -i \left( \Theta(t) \, \langle e^{iHt} \, h_{\alpha,q} \, e^{-iHt} \, h_{\alpha,q}^\dagger \rangle - \Theta(-t) \, \langle h_{\alpha,q}^\dagger \, e^{iHt} \, h_{\alpha,q} \, e^{-iHt} \rangle \right) = -i \, \Theta(t) \, \langle h_{\alpha,q}(t) \, h_{\alpha,q}^\dagger \rangle \]

It follows that

\[ G_\alpha(q, \omega) = \int_0^\infty dt \, e^{i\omega t} \, G_\alpha(q, t) \]

is analytic in the upper \( \omega \)-half plane: Let

\[ \omega = \omega' + i\omega'' \Rightarrow e^{i\omega t} = e^{i\omega' t} \, e^{-\omega'' t} \]

⇒ The hole Green’s function \( G_\alpha(q, \omega) \) is analytic in the upper \( \omega \) half-plane
Now we can perform the integral over $\nu$

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

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

\[
\Sigma_a(k, \omega) = (-2\pi i) \frac{i}{2\pi} \frac{2}{N} \sum_q M^2(k, q) G_b(k - q, \omega - \omega_q)
\]
We had

\[ \Sigma_a(k, \omega) = \frac{2}{N} \sum_q M^2(k, q) G_b(k - q, \omega - \omega_q) \]

and

\[ G_a(k, \omega) = \frac{1}{\omega - \Sigma_a(k, \omega)} \]

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

\[ \Sigma(k, \omega) = \frac{2}{N} \sum_q \frac{M^2(k, q)}{\omega - \omega_q - \Sigma(k - q, \omega - \omega_q)} \]

With

- \( M(k, q) = \epsilon_{k-q} u_q - \epsilon_k v_q \)
- \( \omega_q = \frac{zJ}{2} \sqrt{1 - \gamma_q^2} \)

This is a self-consistency equation for \( \Sigma(k, \omega) \) which has to be solved numerically for a discrete \( k- \) and \( \omega- \) mesh.
Dispersion of the ‘quasiparticle peak’ from the SCBA compared to Lanczos

- Width of lower Hubbard band $4t \to 0.6t$ - actually the bandwidth is $\propto J$
- Change of dispersion - maximum shifted $(\pi, \pi) \to (\frac{\pi}{2}, \frac{\pi}{2})$
- Bulk of spectral weight shifted to incoherent continua
- All in all: massive change of the photoemission spectrum
Comparison with experiment: ARPES spectra for Sr$_2$CuO$_2$Cl$_2$ (B. O. Wells et al., PRL 74, 964 (1995))

By adding $t'$ and $t''$ one can obtain good agreement (O. Sushkov et al., PRB, 56, 11769 (1997))

Summary: Problems to be solved

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

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

Perhaps a phase transition between two phases of different Fermi surface volume?
Does one see anything like this in experiment?
Does one see anything like this in experiment?
Transport properties also are consistent with a ‘small’ Fermi surface

(Data from W. J. Padilla et al., PRB 72,060511 (2005) - remember: \( n_e = 1 - x \))
Does one see anything like this in experiment?

Possible Scenario
Question: Which ‘true’ behaviour might the Hubbard-I approximation be ‘trying to approximate’?

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