Lecture notes: Fermi-Hubbard model

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I. CRYSTALLOGRAPHIC POTENTIAL

   Consider a nonrelativistic particle in a crystallographic periodic potential with period a. For simplicity, we will treat this problem in 1+1 dimensions. Let us begin by writing down the single-particle Hamiltonian

   \[ H = -\frac{\hbar^2}{2m} \partial_{xx} + V_{\text{crys.}}(x), \] (1)

   where \( V_{\text{crys.}}(x) = V_{\text{crys.}}(x + a). \)

   A. Bloch waves and quasimomentum

   The eigenstates of (1) may be written in the form

   \[ \phi_k^{(n)}(x) = e^{ikx} u_k^{(n)}(x), \] (2)

   where \( u_k^{(n)}(x) = u_k^{(n)}(x + a) \) is a periodic function known as the Bloch wave for the crystal and where \( k \) is a real-valued wave number. Since

   \[ -\partial_{xx} \phi_k^{(n)}(x) = 2 e^{ikx} (\partial_x - 2ik \partial_x + k^2) u_k^{(n)}(x), \] (3)

   and since

   \[ (i\partial_x + k)^2 = -\partial_{xx} - 2ik \partial_x + k^2 \] (4)

   the energy eigenvalue

   \[ H \phi_k^{(n)}(x) = E_k^{(n)} \phi_k^{(n)}(x) \] (5)

   reduces to an equation the Bloch waves

   \[ \left( \frac{-i\hbar \partial_x + \hbar k}{2m} + V_{\text{crys.}}(x) \right) u_k^{(n)}(x) = E_k^{(n)} u_k^{(n)}(x), \] (6)

   where \( \hbar k \) is called the quasimomentum of the crystallographic potential. The wave number range \( k \in (\pi/2, \pi/a] \) defines the primitive cell in reciprocal space\(^1\), also known

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\(^1\) The wave number \( k \)-space (the Fourier transform of position \( x \)-space) is called reciprocal space in the condensed matter literature.
as the first Brillouin zone. The eigenvalue problem has a family of solutions (a discrete energy spectrum) labelled by the quantum number \( n \) for each wave number \( k \). The Bloch wave solutions \( u_k^{(n)}(x) \) represents the band structure of the crystal with energy bands \( E_k^{(n)} \).

B. Sine squared potential

Let us consider a scalar quantum particle in a sine squared potential

\[
V_{\text{crys}}(x) = V_0 \sin^2(kx) . \tag{7}
\]

Then [1] may be written as

\[
-\frac{\hbar^2}{2m} \frac{\partial^2 \phi_k^{(n)}}{\partial x^2} + V_0 \left( 1 - \cos 2kx \right) \frac{\phi_k^{(n)}}{2} = E_k^{(n)} \phi_k^{(n)} , \tag{8a}
\]

which after rescaling \( x \rightarrow kx \equiv w \) becomes a differential equation in \( w \) for the function \( y(w) \equiv \phi_k^{(n)}(kx) \)

\[
-\frac{\hbar^2 k^2}{2m} \frac{\partial^2 y}{\partial w^2} + V_0 \left( 1 - \cos 2w \right) y = E_k^{(n)} y . \tag{8b}
\]

With the atomic recoil energy \( E_R \equiv \hbar^2 k^2/(2m) \), the eigenequation may be written as Mathieu’s differential equation

\[
\partial_{ww} y + \left[ a - 2q \cos(2w) \right] y = 0 , \tag{8c}
\]

with constant coefficients

\[
a \equiv \frac{E_k^{(n)} - V_0/2}{E_R} , \tag{9a}
\]

\[
q \equiv -\frac{V_0}{4E_R} . \tag{9b}
\]

According to Floquet’s theorem, any Mathieu function (i.e. solution to \( 8c \)) can be written in the form

\[
y(w) = e^{irw}f(w) , \tag{10}
\]

where \( f(w) \) has period \( 2\pi \) and the integer-valued parameter \( r \) is known as the Mathieu exponent. This is the mathematician’s version of the physicist’s Bloch wave solution with quasimomentum \( rk \) discussed above.

An example Bloch wave solution is shown in Fig. 1. The band structure of the quantum particle is shown in Fig. 2 for the lowest three energy eigenstates. Band gaps appear and then widen as the \( V_0 \) increases. For very large \( V_0 \) the bands become flat (i.e. the band width of each energy band approaches zero and the forbidden energy regions become maximally large).

C. Localized Wannier functions

The advantage of the Bloch wave solutions is that they represent orthogonal energy eigenstates. However, they are delocalized states. If one is interested in localized orthogonal states\(^2\), then these can be constructed as a superposition of Bloch waves

\[
w_n(x - x_i) = \frac{1}{2N} \sum_{\nu=-N}^{N-1} e^{-ik_{\nu}x_i}\phi_k^{(n)}(x) , \tag{11}
\]

\(^2\) A localized state is one where the quantum particle’s wave function is narrow and primarily positioned near the minimum of one well in the periodic potential. The quantum particle’s average position is centered at the well’s minimum.
for \( k_v = \pi \nu / (Na) \) with a crystal size \( a \). Such localized states are Wannier functions [Wannier 1937] when we make the assumption that the Bloch wave is independent of wave number. Hence, writing the energy eigenstate as \( \phi^{(n)}(x) = e^{ik_v x} u(0)(x) \), then we express the Wannier functions as

\[
\psi_n(x - x_i) = \frac{u^{(0)}(x)}{2N} \sum_{\nu = -N}^{N-1} e^{i k_v (x - x_i)} \tag{12a}
\]

\[
= \frac{u^{(0)}(x)}{2N} \sum_{\nu = -N}^{N-1} e^{i \frac{\pi \nu}{Na} (x - x_i)} \tag{12b}
\]

We can make use of finite geometric series identity

\[
\frac{1}{N} \sum_{\nu = -N}^{N-1} z^n = \frac{1}{N} \frac{z^N - z^{-N}}{z - 1} \tag{13}
\]

to rewrite (12b) as

\[
\psi_n(x - x_i) = \frac{u^{(0)}(x)}{2N} \frac{e^{i \pi \nu / Na} (x - x_i) - e^{-i \pi \nu / Na} (x - x_i)}{e^{i \pi / Na} (x - x_i) - 1} \tag{14a}
\]

\[
= \frac{i u^{(0)}(x)}{N} \frac{\sin(\pi (x - x_i)/a)}{e^{i \pi / Na} (x - x_i) - 1} \tag{14b}
\]

\[
= u^{(0)}(x) \frac{\sin(\pi (x - x_i)/a)}{\pi (x - x_i)/a} + \cdots \tag{14c}
\]

\[
\approx u^{(0)}(x) \text{sinc}(\pi (x - x_i)/a) \tag{14d}
\]

which is indeed a localized wave packet centered at \( x_i \).

II. ONE-BAND HUBBARD HAMILTONIAN

Here we briefly review the one-band Hubbard model [Hubbard 1967] that describes a system of spin one-half fermions on a lattice by the Hamiltonian

\[
H = -t \sum_{\langle ij \rangle \sigma} \left( a^\dagger_{i\sigma} a_{j\sigma} + a^\dagger_{j\sigma} a_{i\sigma} \right) + U \sum_i n_{i\uparrow} n_{i\downarrow} + U \sum_{i\sigma} n_{i\sigma}, \tag{15}
\]

where \( a^\dagger_{i\sigma} \) and \( a_{i\sigma} \) are the Wannier fermionic creation and destruction operators creating and destroying an electron of spin \( \sigma \) at site \( i \) of the lattice.

The physical meaning of each term comprising the Hubbard Hamiltonian is straightforward. The first term of (15), the kinetic energy, accounts for electron tunneling from site \( j \) to site \( i \) and thereby reduces the energy of the system by a factor \( t \) for each tunneling event. The site summation denoted by \( \langle ij \rangle \) is over all bonds of the lattice. In our investigation we restrict ourselves to nearest-neighbor tunneling or hopping. The interaction part of the Hubbard Hamiltonian accounts for the Coulomb interaction between two electrons residing on the same site and therefore is a simplification of the full Coulomb interaction term

\[
H^{\text{int}} = \int d^3r d^3r' \hat{\psi}^\dagger(r) \hat{\psi}(r) V(r - r') \hat{\psi}^\dagger(r') \hat{\psi}(r'), \tag{16}
\]

where \( \hat{\psi}(r) \) is the field operator at the space point \( r \). The last two terms of (15) are obtained from (16) if one substitutes for the field operator a linear combination of Wannier states, denoted \( \phi_{i\sigma}(r) \), as follows,

\[
\psi(r) = \sum_{i\sigma} a_{i\sigma} \phi_{i\sigma}(r). \tag{16}
\]

Denotes the intra-site matrix elements of the Wannier states so that the significant short-ranged part of the Coulomb interaction is modeled. Then (16) reduces to

\[
H^{\text{int}} = U \sum_{i\sigma} n_{i\sigma} n_{i\sigma} = U \sum_i n_{i\uparrow} n_{i\downarrow} + U \sum_{i\sigma} n_{i\sigma}^2. \tag{17}
\]

The last term of (17) is a constant self-energy, \( UN_c \), where \( N_c \) is the total number of electrons, because \( n_{i\sigma}^2 = n_{i\sigma} \) for fermions. Since this term only causes a constant energy shift of the spectrum it is typically ignored.

Obtaining analytic solutions of the Hubbard model is difficult. Exact solutions are possible for certain cases, for example when \( U/t = 0 \) or when \( U/t = \infty \), the latter being the strong-coupling limit where doubly occupied sites are prohibited. A well known approximation approach involves altering the Hubbard Hamiltonian by a unitary transformation to express it in a \( t/U \) expansion [Gros et al. 1987]. The lowest order terms of this expansion are kept in the large-\( U \) limit, both large on-site mutual interaction and self-interaction. This is the \( t-J \) model.

Here we shall focus on exact solutions. As a first exercise toward understanding strongly-correlated Fermi matter governed by the Hubbard Hamiltonian, we now consider exact solutions of (15) for small clusters.

A. Method of solution

Here we demonstrate our quantum information method by applying it to the one-band Hubbard model for small clusters. As examples, we consider the triangular and square clusters. We implement operators used to diagonalize the Hamiltonian with respect to symmetry and total-spin. Joint number operators are employed to represent a swap gate which in turn is used to represent a fermionic interchange operator and the total-spin-squared operator. Finally, we implement the second quantized form of Wannier creation and annihilation operators in terms of qubit creation and annihilation operators in a numbered state representation.

1. Block diagonalization

The first step in solving the Hubbard model for small clusters, given a lattice of size \( L \) and number of electrons \( N_e \), is to determine a set of basis states. Since the \( z \)-component of the spin commutes with the Hamiltonian, we have chosen to work with a set of basis states in the number representation with a given \( S_z \). This is done for convenience since one can immediately determine \( S_z \) for any such state by inspection. Throughout the remainder
of this lecture we shall denote an $S_z$ basis by the symbol \{\phi_n\}.

As an example of the size of the basis, in the case of half filling, where $N_e = L$ and $S_z = 0$, for the triangular and square clusters there are 9 and 36 states, respectively.

The triangular cluster possesses the $C_{3v}$ point group symmetry and the square $C_{4v}$.

**TABLE I** $C_3$ (with $\epsilon = e^{i\pi/3}$) and $C_{3v}$ character tables.

<table>
<thead>
<tr>
<th>$C_3$</th>
<th>$E$</th>
<th>$C_3$</th>
<th>$C_3'$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A$</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>$E$</td>
<td>$\epsilon$</td>
<td>$\epsilon^*$</td>
<td>$\epsilon$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$C_{3v}$</th>
<th>$E$</th>
<th>$2C_3$</th>
<th>$3\sigma_v$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_1$</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>$A_2$</td>
<td>1</td>
<td>1</td>
<td>-1</td>
</tr>
<tr>
<td>$E$</td>
<td>2</td>
<td>-1</td>
<td>0</td>
</tr>
</tbody>
</table>

**TABLE II** $C_4$ and $C_{4v}$ character tables.

<table>
<thead>
<tr>
<th>$C_4$</th>
<th>$E$</th>
<th>$C_4$</th>
<th>$C_4'$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A$</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>$B$</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
</tr>
<tr>
<td>$C$</td>
<td>$i$</td>
<td>-1</td>
<td>-1</td>
</tr>
<tr>
<td>$E$</td>
<td>$i$</td>
<td>-1</td>
<td>1</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$C_{4v}$</th>
<th>$E$</th>
<th>$2C_4$</th>
<th>$C_2$</th>
<th>$2\sigma_v$</th>
<th>$2\sigma_d$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_1$</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>$A_2$</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td></td>
</tr>
<tr>
<td>$B_1$</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
<td></td>
</tr>
<tr>
<td>$B_2$</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>$E$</td>
<td>2</td>
<td>0</td>
<td>-2</td>
<td>0</td>
<td></td>
</tr>
</tbody>
</table>

The second step is to determine matrices representing the point group operations in the basis \{\phi_n\}. This is accomplished by successively employing site-interchange operations, as detailed below, to rotate or reflect any particular state according to the appropriate group operation desired. Let us denote these various operations by the generic symbol $R$. The $C_{3v}$ group has six group operations and three irreducible representations, and $C_{4v}$ has eight and five, respectively; see Table I and Table II.

Let us denote the $i$th irreducible representations by $\Gamma_i$. Given that we have constructed a reducible matrix representation, denoted $M_{mn}^R$, of the symmetry group in our basis \{\phi_n\}, we then construct projection operators, denoted $P_{mn}^R$, for each of the irreducible representations of the group \cite{Chen1988, Freericks1991, Reich1988}.

Below, we shall denote a total spin-squared basis by the symbol $\varphi_m^{S^2}$. Since $S^2$ commutes with the Hamiltonian we thereby partition each symmetry block into smaller blocks, each having a definite total spin eigenvalue $S$.

The final step is to calculate the matrix elements of the Hubbard Hamiltonian in the $\varphi_m^{S^2}$ basis, and analytically find, if possible, the eigenvalues and eigenvectors of each resulting spin-and-symmetry block and thereby complete the analytical solution. In the case of the triangle, the largest $\varphi_m^{S^2}$ block is $3 \times 3$ and for the square it is $4 \times 4$. So these two clusters are analytically tractable.

In summary, we denote the various sectors of the Hilbert space with quantum state symbols given by

$$
\frac{N_e \phi_{N_e,S_z} | \Gamma_i | S^2}{\psi_{S_i}^{S_i}},
$$

for integer $N_e \in [0, 6]$ and for $S_z = 0, \pm \frac{1}{2}, \pm 1, \pm \frac{3}{2}$ and for $i \in \{A_1, A_2, E\}$ of the $C_{3v}$ point group for the $L = 3$ lattice (triangular cluster) and for integer $N_e \in [0, 8]$ and for $S_z = 0, \pm \frac{1}{2}, \pm 1, \pm \frac{3}{2}, \pm 2$ and for $i \in \{A_1, A_2, B_1, B_2, E\}$ of the $C_{4v}$ point group for the $L = 4$ lattice (square cluster).

An important point must be mentioned here. We have found using projection operators constructed from the $C_3$ and $C_4$ character tables breaks the size of the $E$-type blocks in two for the half-filled cases.
2. Site interchange operator

We can use the qubit creation and annihilation operators, $a_i^\dagger$ and $a_i$, for the $i$th qubit, to represent Wannier spin creation and annihilation operators, $a_i^\dagger_{\sigma}$ and $a_i^\dagger_{\overline{\sigma}}$ for the spin component (say along the z-axis) of value $\sigma$, at the $i$th lattice point. Two qubits are required to encode one quantum spin-position state, both having four basis states per point. The isomorphism between the Wannier and qubit operators are mapped as follows ($i = 1, \ldots, L^D$):

<table>
<thead>
<tr>
<th>Wannier operator</th>
<th>qubit operator</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a_i^\dagger$</td>
<td>$a_{2i-1}^\dagger$</td>
</tr>
<tr>
<td>$a_i$</td>
<td>$a_{2i-1}$</td>
</tr>
<tr>
<td>$a_i^\dagger$</td>
<td>$a_{2i}$</td>
</tr>
<tr>
<td>$a_i$</td>
<td>$a_{2i}$</td>
</tr>
</tbody>
</table>

We use the following bit encoding and notation for the electrons at a point:

- $|e\rangle = |00\rangle$, $0$ (empty)
- $|p\rangle = |01\rangle$, $e^-_i$ (plus or spin-up)
- $|m\rangle = |10\rangle$, $e^+_i$ (minus or spin-down)
- $|d\rangle = |11\rangle$, $e^+_i e^+_i$ (double).

All symmetry operations of rotation or reflection are implemented by a particular successive application of a fermionic interchange operator, which we denote by $\chi_{ij}$ where the interchange of electrons occurs between sites $i$ and $j$.

$\chi_{ij}$ may be implemented using SWAP gates and the following is one derivation of its unitary form in terms of Wannier creation and annihilation operators. We wish to construct $\chi_{ij}$ so to correctly handle any necessary phase change due to the fermion anticommutation relations. The simplest implementation of $\chi_{ij}$ should involve only products of $a_i^\dagger_\alpha$ and $a_i^\dagger_{\overline{\alpha}}$.

For an site interchange operator, we require that $\chi_{ij}^2 = 1$, that the site interchange operator conserve the number of particles, $[\chi_{ij}, N] = 0$, that $\chi_{ij}$ is hermitian, and that $\chi_{ij}|0\rangle = |0\rangle$. Let us assume we have a one-particle state $\phi_{1e} = a^\dagger_{\sigma m}|0\rangle$ where $m = i$ or $j$. A first guess at the analytical form of a spin-dependent SWAP gate between sites $i$ and $j$ would be

$$\chi_{ij} = a_{j\sigma}^\dagger a^\dagger_{i\overline{\sigma}} + a^\dagger_{i\overline{\sigma}} a_{j\sigma}.$$  (24)

This acts correctly on $\phi_{1e}$. The problem with (24) is that its application on to the vacuum violates our requirement that $\chi_{ij}|0\rangle = |0\rangle$. This is remedied easily enough by slightly modifying our first guess

$$\chi_{ij} = a^\dagger_{i\sigma} a_{i\sigma} + a^\dagger_{j\sigma} a_{j\sigma} + 1.$$  (25)

Although (25) repairs the vacuum problem, now its application onto $\phi_{1e}$ would interchange the electron but incorrectly would also give back $\phi_{1e}$, an extra unwanted electron. We administer the final remedy by including two more terms that have the effect of subtracting off the unwanted electron

$$\chi_{ij\sigma} = a^\dagger_{j\sigma} a_{i\sigma} + a^\dagger_{i\sigma} a_{j\overline{\sigma}} + 1 - a^\dagger_{i\overline{\sigma}} a_{i\overline{\sigma}} - a^\dagger_{j\sigma} a_{j\sigma}.$$  (26)

Although we have constructed (26) by considering only a one-particle state, a remarkable fact is that $\chi_{ij\sigma}$ works on any arbitrary state.

Let us investigate the structure of $\chi_{ij\sigma}$ further. Let us rewrite (26) by factoring the creation operators,

$$\chi_{ij\sigma} = 1 + a^\dagger_{j\sigma} (a_{i\sigma} - a_{j\sigma}) + a^\dagger_{i\sigma} (a_{j\sigma} - a_{i\sigma}),$$  (27)

which leads one to write

$$\chi_{ij\sigma} = 1 - (a^\dagger_{j\sigma} - a^\dagger_{i\sigma})(a_{j\sigma} - a_{i\sigma}).$$  (28)

Now of course, one is motivated to define the following joint creation, annihilation, and number operators

$$A_{ij\sigma} = \sqrt{\frac{1}{2}} (a_{j\sigma} - a_{i\sigma})$$  (29)

$$A^\dagger_{ij\sigma} = \sqrt{\frac{1}{2}} \left( a^\dagger_{i\overline{\sigma}} - a^\dagger_{j\overline{\sigma}} \right)$$  (30)

$$N_{ij\sigma}^A = A^\dagger_{ij\sigma} A_{ij\sigma}$$  (31)

so that (26) may be written as

$$\chi_{ij\sigma} = 1 - 2 N_{ij\sigma}^A.$$  (32)

Our joint operators work in a number representation formed of entangled states

$$A^\dagger_{ij\sigma}|\sigma\rangle = \sqrt{\frac{1}{2}} \left( |j\sigma\rangle - |i\sigma\rangle \right) \equiv |A_{ij\sigma}\rangle.$$  (33)

The joint number operator satisfies $(N_{ij\sigma}^A)^2 = N_{ij\sigma}^A$ and consequently we have

$$\chi_{ij\sigma}^2 = (1 - 2 N_{ij\sigma}^A)^2 = 1 - 4 N_{ij\sigma}^A + 4 N_{ij\sigma}^A^2 = 1,$$  (34)

satisfying another of our requirements.

It can be written in exponential form

$$\chi_{ij\sigma} = e^{\pm N_{ij\sigma}^A},$$  (35a)

$$\chi_{ij\sigma} = 1 + z N_{ij\sigma}^A + \frac{z^2}{2!} N_{ij\sigma}^A + \cdots$$  (35b)

$$\chi_{ij\sigma} = 1 + (z + \frac{z^2}{2!} + \cdots) N_{ij\sigma}^A$$  (35c)

$$\chi_{ij\sigma} = 1 + (e^z - 1) N_{ij\sigma}^A.$$  (35d)

Comparing (32) with (35a), allows us to choose $z = \pi i$, so we have our SWAP gate

$$\chi_{ij\sigma} = \chi_{ij\sigma} = e^{i \pi N_{ij\sigma}^A},$$  (36)
which are 120° appearing as a rotation by 180°.

To affect the interchange of electrons between the sites \(i\) and \(j\), one defines the site interchange operator as the product operator

\[
\chi_{ij} \equiv \chi_{ij1}\chi_{ij1}.
\]  

(37)

For the triangular cluster, we implement the \(C_{3v}\) point operators as follows:

\[
R^{C_3} = \chi_{12}\chi_{23}
\]  

(38a)

\[
R^{C_2} = \chi_{23}\chi_{12}
\]  

(38b)

\[
R^{\sigma(1)} = \chi_{23}
\]  

(38c)

\[
R^{\sigma(2)} = \chi_{31}
\]  

(38d)

\[
R^{\sigma(3)} = \chi_{12},
\]  

(38e)

which are 120° and 240° rotations, and reflections about sites 1, 2, and 3, respectively. For the square cluster, we implement the \(C_{4v}\) point group operators as follows:

\[
R^{C_4} = \chi_{34}\chi_{23}\chi_{12}
\]  

(39a)

\[
R^{C_2} = \chi_{23}\chi_{12}
\]  

(39b)

\[
R^{C_3} = \chi_{12}\chi_{23}\chi_{34}
\]  

(39c)

\[
R^{\sigma(1)} = \chi_{24}
\]  

(39d)

\[
R^{\sigma(2)} = \chi_{13}
\]  

(39e)

\[
R^{\sigma(3)} = \chi_{12}\chi_{34}
\]  

(39f)

\[
R^{\sigma(4)} = \chi_{14}\chi_{23},
\]  

(39g)

which are 90°, 180° and 270° rotations, and reflections about two diagonals and the vertical and horizontal, respectively.

3. Implementation of the \(S^2\) operator

The site-specific total-spin operator is compactly written in terms of the Wannier creation and annihilation operators and the Pauli spin matrices as

\[
S_i = \frac{1}{2} \sigma_{\alpha\beta} a_{i\alpha}^\dagger a_{i\beta},
\]  

(40)

where \(h = 1, \sigma = (\sigma_x, \sigma_y, \sigma_z)\), and

\[
\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.
\]

The components of (40) are then

\[
S_{ix} = \frac{1}{2} \sigma_{\alpha\beta} a_{i\alpha}^\dagger a_{i\beta} + \frac{1}{2} a_{i\alpha}^\dagger a_{i\beta}^\dagger,
\]  

(41a)

\[
S_{iy} = \frac{1}{2} \sigma_{\alpha\beta} a_{i\alpha}^\dagger a_{i\beta} = \frac{i}{2} a_{i\alpha}^\dagger a_{i\beta}^\dagger + a_{i\beta}^\dagger a_{i\alpha}^\dagger,
\]  

(41b)

\[
S_{iz} = \frac{1}{2} \sigma_{\alpha\beta} a_{i\alpha}^\dagger a_{i\beta} = \frac{1}{2} \left( a_{i\alpha}^\dagger a_{i\beta}^\dagger - a_{i\beta}^\dagger a_{i\alpha}^\dagger \right).
\]  

(41c)

Using the mapping (22), the spin operators may be expressed in terms of the qubit creation and annihilation operators

\[
S_{ix} = \frac{1}{2} \left( a_{2i-1}^\dagger a_{2i} + a_{2i}^\dagger a_{2i-1} \right),
\]  

(42a)

\[
S_{iy} = \frac{i}{2} \left( -a_{2i-1}^\dagger a_{2i} + a_{2i}^\dagger a_{2i-1} \right),
\]  

(42b)

\[
S_{iz} = \frac{1}{2} \left( a_{2i-1}^\dagger a_{2i} - a_{2i}^\dagger a_{2i-1} \right).
\]  

(42c)

Then, the the spin along \(\hat{z}\) of the numbered state is

\[
S_z = \sum_{i=1}^{L} S_{iz},
\]  

(43)

where \(S_z\varphi = S_z\varphi\). Furthermore, the square of the total spin operator is readily constructed

\[
S^2 = \sum_{i=1}^{L} \sum_{j=1}^{L} \left( S_{ix}S_{jx} + S_{iy}S_{jy} + S_{iz}S_{jz} \right),
\]  

(44)

where \(S^2\varphi = S(S+1)\varphi\). We use the eigenvalues \(S_z\) and \(S\) as good quantum numbers to specify the quantum state of the system.

B. Exact solutions

Here we analyze our findings for the triangular and square cluster tabulated in Appendices A and B. We evaluate these solutions for the expected symmetries of the Hubbard Hamiltonian and find that the method leads to consistent results. We check a theorem proved by Nagaoka concerning whether or not the ferromagnetic state above and below half filling is the ground state. Then, we compare spin-correlations of the ground states of the triangular and square clusters at half filling. Finally we give some examples and interpretation of eigenvalue and photoemission energies as a function of \(U/t\).
1. Double-empty symmetry above and below half filling

It is well known that, energetically, the Hubbard Hamiltonian possesses a symmetry above and below half filling. This symmetry ensures a one-to-one correspondence between states above half filling with those below. The structure of the states, their exact symmetry and total-spin, above and below half filling is identical provided that the respective $S_z$ basis, $\{\phi_n\}$, are labeled so that any state above half filling with a particular doubly occupied site corresponds to a state below half filling with no electrons on that site.

Let us consider the solutions for the triangular cluster and, further, consider the cases with $S_z = 0$ above and below half filling, presented in Sec. A.2 and Sec. A.4. The first point to note is that $\{\psi^n_{N_z=1,S_z=0}\}$ can be mapped to $\{\psi^n_{N_z=2,S_z=0}\}$ by taking $d \to e$. The structure of the states are seen to be identical by comparing the eigenkets in Sec. A.2 to those in Sec. A.4. Finally, the energies are also seen to be isomorphic by taking $t \to -t$ and if, above half filling, we shift the energy down by $3U$. The origin of this shift is two-fold: (a) the second term of the Hubbard Hamiltonian [15] causes a shift of $U$ since $d \to e$; and (b), the third term of the Hamiltonian (self energy) causes a shift of $2U$ in our case. The same symmetry is seen to exist for the cases with $S_z = 1$; see Sec. A.3 and A.5.

For the case of the square cluster this symmetry is essentially the same, differing only in that the asymmetry in $t$ is not present. The underlying reason for difference between the triangle and square arises from the freedom we have to divide the square into two sublattices such that for any lattice point has nearest-neighbors belonging to the co-sublattice [Nagaoka 1966]. Then a phase difference of $-1$ between the wave function of the sublattices accounts for a change in the sign of $t$.

2. Check of Nagaoka’s theorem

Let us consider the triangular cluster below half filling, $N_e = 2$. The ground state of this system could have either $S_z = 0$ or 1. In the $S_z = 0$ case, the numbered basis states are

$$
\begin{align*}
\phi_1 &= |\text{emp}\rangle \\
\phi_2 &= |\text{pem}\rangle \\
\phi_3 &= |\text{mpe}\rangle \\
\phi_4 &= |\text{emp}\rangle \\
\phi_5 &= |\text{mpe}\rangle \\
\phi_6 &= |\text{mpe}\rangle. \\
\phi_7 &= |\text{ede}\rangle \\
\phi_8 &= |\text{ede}\rangle \\
\phi_9 &= |\text{eed}\rangle.
\end{align*}
$$

In this $\{\phi\}$ basis, the matrix elements of the A1 symmetry operator

$$
\Gamma_{A1} = \frac{1}{6} \left( 1 + R^{C1} + R^{C2} + R^{C3} + R^{C3} + R^{C3} \right)
$$

are

$$
\langle \phi_i | \Gamma_{A1} | \phi_j \rangle = \frac{1}{6} \begin{pmatrix}
1 & -1 & 1 & -1 & 1 & -1 & 0 & 0 & 0 \\
-1 & 1 & -1 & 1 & -1 & 1 & 0 & 0 & 0 \\
1 & -1 & 1 & -1 & 1 & -1 & 0 & 0 & 0 \\
1 & -1 & 1 & -1 & 1 & -1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 2 & 2 & 2 \\
0 & 0 & 0 & 0 & 0 & 0 & 2 & 2 & 2 \\
0 & 0 & 0 & 0 & 0 & 0 & 2 & 2 & 2
\end{pmatrix}_{ij}.
$$

From this result, we see that the $\{\psi\}$ basis is

$$
\psi_1 = \frac{1}{\sqrt{6}} \left( |\text{emp}\rangle - |\text{pem}\rangle + |\text{mpe}\rangle + |\text{empe}\rangle - |\text{pem}\rangle - |\text{mpe}\rangle \right)
$$

$$
\psi_2 = \frac{1}{\sqrt{3}} \left( |\text{ede}\rangle + |\text{ede}\rangle + |\text{eed}\rangle \right),
$$

which are antiferromagnetic states. The lowest energy eigenstate in the $N_e = 2$ and $S_z = 0$ sector has $A_1$ symmetry and total spin $S = 0$. In the $\{\psi\}$ basis, the matrix elements of the Hubbard Hamiltonian are

$$
\langle \psi_i | H | \psi_j \rangle = \frac{-2t}{2\sqrt{2t}} \begin{pmatrix}
2 \sqrt{t} & U
\end{pmatrix}_{ij}.
$$

In comparing (50) with (A10) presented in Appendix A note that we have subtracted $2U$ (self-energy) from the diagonals of the matrix elements for simplicity. Diagonalizing (50), we find the exact solution for the lowest energy eigenstates to be

$$
\Psi_{A_1}^{S_z=0,S=0} = \frac{\alpha}{\sqrt{6}} \left( |\text{emp}\rangle - |\text{pem}\rangle - |\text{mpe}\rangle - |\text{pem}\rangle - |\text{mpe}\rangle \right)
$$

$$
+ \frac{\beta}{\sqrt{3}} \left( |\text{ede}\rangle + |\text{ede}\rangle + |\text{eed}\rangle \right),
$$

where the normalized coefficients $\alpha$ and $\beta$ are

$$
\begin{align*}
\alpha &= \frac{\mu}{\sqrt{1 + \mu^2}} \quad (52a) \\
\beta &= \frac{1}{\sqrt{1 + \mu^2}} \quad (52b)
\end{align*}
$$

with

$$
\mu = -\frac{2t + U \pm \sqrt{36t^2 + 4tU + U^2}}{4\sqrt{2t}}.
$$

The coefficients $\alpha$ and $\beta$ (for the positive root in $\mu$) are plotted in Fig. 4b, for unity hopping coefficient $t = 1$.

In the $S_z = 1$ case, the lowest energy state, the ferromagnetic state, has $E$ symmetry and total spin $S = 1$

$$
\Psi_{S_z=1,S=1} = \frac{1}{\sqrt{3}} (2|\text{cpp}\rangle + |\text{pem}\rangle - |\text{pme}\rangle) = \frac{1}{\sqrt{3}} (2|\text{cpp}\rangle + |\text{pem}\rangle - |\text{pme}\rangle) / \sqrt{3}
$$

$$
\langle H_{S_z=1}^E \rangle = -t,
$$

$$
\langle H_{S_z=1}^E \rangle = -t.
$$
where again we have subtracted 2U (the self-energy). We see in Fig. 4a that below half filling the ferromagnetic state is not the ground state of the system for all values of U. Nagaoka has proven, in the limit \( U \rightarrow \infty \), for an fcc or hcp lattice that the ferromagnetic state with the maximum total spin would not be the ground state of the system \([\text{Nagaoka} 1966]\). Our results are in agreement with this statement, if we make an analogy between our triangular cluster and fcc or hcp.

Let us see in more detail why \( \Psi_{A_{12},S=0}^{S_z=0,S=0} \) is indeed the ground state of the system. Let us consider the \( U = 0 \) limit. Here the Hubbard Hamiltonian has only the kinetic energy term

\[
\mathcal{H}_o = -t \sum_{\langle ij \rangle, \sigma} \left( a_{i\sigma}^\dagger a_{j\sigma} + a_{j\sigma}^\dagger a_{i\sigma} \right)
\]

which we can transform to \( k \)-space to determine the band energy. To convert from Bloch states (in reciprocal space) to Wannier states (in position space) we use the discrete inverse Fourier transform

\[
a_{i\sigma} = \frac{1}{N} \sum_k e^{-ikR_i} a_{k\sigma} \quad \quad a_{i\sigma}^\dagger = \frac{1}{N} \sum_k e^{ikR_i} a_{k\sigma}^\dagger \tag{56a}
\]

and to go from position space back to reciprocal space we use the discrete Fourier transform

\[
a_{k\sigma} = \sum_{\{R_i\}} e^{ikR_i} a_{i\sigma} \quad \quad a_{k\sigma}^\dagger = \sum_{\{R_i\}} e^{-ikR_i} a_{i\sigma}^\dagger \tag{56b}
\]

where the possible momenta are \( k = k_n = 2n\pi/Na \) and lattice vectors are \( R_n = an, \quad n = 0,1, \ldots, N-1 \) and \( a \) is the cellsize. Substituting (56a) into (55) gives

\[
\mathcal{H}_o = -t \sum_{\langle ij \rangle, \sigma} \left( a_{i\sigma}^\dagger a_{j\sigma} + a_{j\sigma}^\dagger a_{i\sigma} \right)
\]

where we have gone from (57a) to (57b) by replacing the sum over the bonds, \( \langle ij \rangle \), by a sum only over the lattice sites since for nearest-neighbor interactions, \( R_j = R_i \pm a \) in the \( \langle ij \rangle \) sum. We then have

\[
\mathcal{H}_o = \sum_{k\sigma} \epsilon_k a_{k\sigma}^\dagger a_{k\sigma}, \tag{58}
\]

where \( \epsilon_k = -2t \cos ka \) and where we have used

\[
\frac{1}{N} \sum_i e^{i(k-k')R_i} = \delta_{kk'} \tag{59}
\]

Referring to Fig. 5a and Fig. 5b, clearly for \( N_c = 2 \) the \( S_z = 0 \) energy eigenstate has lowest energy eigenvalue, \(-4t\), while the \( S_z = 1 \) energy eigenstate has energy eigenvalue \(-t\). This agrees with Fig. 4a. Let us consider the

\[
\Psi_{A_{12}}^{S_z=0,S=0} \rightarrow \frac{1}{\sqrt{9}} \left( (dee) + |ede\rangle + |ed\rangle \right) - \frac{1}{\sqrt{9}} \left( (emp) - |pem\rangle + |mpe\rangle - |epm\rangle + |mep\rangle - |pme\rangle \right) \tag{61}
\]
the Hubbard Hamiltonian for to the solution (61) obtained by exact diagonalization of $S_{\text{filling}}$ for $S_z = 0, 1$.

3. Quantum informational derivation of the ground state

Remarkably, and as an additional consistency check, we can arrive at (61) much more simply and directly by using an a maximally entangled quantum state that is localized in $k$-space with zero momentum ($k = 0$). That is, we may construct this maximally entangle state, which we can arrive at (61) much more simply and directly by using an a maximally entangled quantum state that is localized in $k$-space with zero momentum ($k = 0$). That is, we may construct this maximally entangle state, which is, we may construct this maximally entangle state, which is formed out of unitary swap gates which by construction have the vacuum as an eigenstate with unity eigenvalue.

where the vacuum state for the $S_z = 0$, $N_e = 2$ creation operators, (56b), as follows:

\[
|a_{k=0}^\dagger a_{k=0}^\dagger|0\rangle = (a_{11}^\dagger + a_{21}^\dagger + a_{31}^\dagger)(a_{11}^\dagger + a_{21}^\dagger + a_{31}^\dagger)|0\rangle
\]  

(62a)

\[
|\text{dee}\rangle + |\text{ede}\rangle + |\text{eed}\rangle
\]

(62b)

\[
- |\text{emp}\rangle + |\text{emp}\rangle - |\text{mp}\rangle - |\text{mp}\rangle + |\text{mp}\rangle + |\text{mp}\rangle,
\]

where the vacuum state for the $L = 3$ is $|0\rangle \equiv |\text{eee}\rangle$. Normalizing this by $\sqrt{3}$, we see that (62) is indeed identical to the solution (61) obtained by exact diagonalization of the Hubbard Hamiltonian for $L = 3$ when we evaluate the exact $(t, U)$-dependent solution at $U = 0$.

The vacuum state $|0\rangle$ may be added in quantum superposition with (62) for the following reasons:

1. it too has quantum numbers $S_z = 0$ and total spin $S = 0$;

2. it too is an eigenstate of $\Gamma_{A1}$, which represents $A1$ symmetry operator$^4$;

3. and it contributes zero energy to the superposition state (i.e. $\langle 0 | H | 0 \rangle = 0$).

Therefore, the $U = 0$ ground state may be written as

\[
\Psi_{A12, U = 0}^{S_z = 0, S_e = 0} = (u + v a_{k=0}^\dagger a_{k=0}^\dagger)|0\rangle,
\]

(63)

where $u$ and $v$ are c-numbers that satisfy the normalization condition

\[
|u|^2 + |v|^2 = 1.
\]

(64)

Therefore, the ground state is superconducting and it contains one Cooper pair. We will explore this generic property of the ground state in the context of large Fermi systems in Lecture 9.

4. Triangular cluster above half filling

Now let us consider the triangular cluster above half filling, $N_e = 4$. Like the case just considered, the ground state of this system could have either $S_z = 0$ or 1. Remarkably, however, in the above half-filled case the ferromagnetic and nonferromagnetic states are degenerate with eigenvalue $5U - 2t$, see Sec. A.2 and A.3. The reason for this degeneracy is depicted in plots (c) and (d) in Fig. 5. The degeneracy arises from the fact that $\epsilon_k = -2t \cos ka$ has the same value for $k = 2\pi/3$ and $k = 4\pi/3$, an effect due to the $L = 3$ cluster.

5. Predicted energy eigenstates for the triangular cluster

Here we give some examples illustrating the insights one may obtain from energy eigenvalue plots. Let us see what physics is contained in an eigenvalue plot such as Fig. 6, where we have plotted all the energies of the half-

\[
\text{Energy}
\]

FIG. 6 Eigenvalues for the triangular cluster at half filling.

filled triangular cluster as a function of $U$. Each curve is labelled according to its symmetry. The $A_1$ and $A_{22}$ energies are degenerate for all $U$. In Fig. 7 we have depicted all the possible Bloch states for $N_e = 3$. There are five types of Bloch states we can possibly choose. These, in turn, correspond to the five nondegenerate energies for finite $U$ plotted in Fig. 6. Consequently, we see why there are only three nondegenerate energies at $U = 0$ in Fig. 6.

---

$^4$ The vacuum is an eigenstate of all the symmetry operators because they are formed out of unitary swap gates which by construction have the vacuum as an eigenstate with unity eigenvalue.
the Bloch states in panels (1), (2), and (3) of Fig. 7 have the same energy at $U = 0$. It is possible to assign each Bloch state a given symmetry. Immediately, we assign panels (1) and (5) of Fig. 7 symmetries $E_1$ and $E_2$, respectively, since they are the highest and lowest energy states. Then, we assign panel (2) $A_{21}$ symmetry since from Fig. 8 the energy of this state is independent of $U$ and we know

$$
\Psi_{A_{21}} = \frac{1}{\sqrt{3}} \left( |mpp\rangle + |pmp\rangle + |ppm\rangle \right). \quad (65a)
$$

Next, we assign panel (3) $A_1$ and $A_{22}$ symmetry since we know that these states must have a doubly occupied site

$$
\Psi_{A_1} = \frac{1}{\sqrt{6}} \left[ (|dpe\rangle + |edp\rangle + |ped\rangle) + (|dep\rangle + |pde\rangle + |epd\rangle) \right], \quad (65b)
$$

$$
\Psi_{A_{22}} = \frac{1}{\sqrt{6}} \left[ (|dpe\rangle + |edp\rangle + |ped\rangle) - (|dep\rangle + |pde\rangle + |epd\rangle) \right]. \quad (65c)
$$

The eigenvalues of the triangular cluster above half filling, $N_e = 4$, and $S_z = 0$ are the following

$$
\lambda_{A_{11}}^{N_e=4,S_z=0} = \frac{11U + 2t + \sqrt{(-11U - 2t)^2 - 4(30U^2 + 12Ut - 8t^2)}}{2}, \quad (66a)
$$

$$
\lambda_{A_{12}}^{N_e=4,S_z=0} = \frac{11U + 2t - \sqrt{(-11U - 2t)^2 - 4(30U^2 + 12Ut - 8t^2)}}{2}, \quad (66b)
$$

$$
\lambda_{A_2}^{N_e=4,S_z=0} = 5U - 2t, \quad (66c)
$$

$$
\lambda_{E_1}^{N_e=4,S_z=0} = 5U + t, \quad (66d)
$$

$$
\lambda_{E_2}^{N_e=4,S_z=0} = \frac{11U - t + \sqrt{(-11U + t)^2 - 4(30U^2 - 6Ut - 2t^2)}}{2}, \quad (66e)
$$

$$
\lambda_{E_3}^{N_e=4,S_z=0} = \frac{11U - t - \sqrt{(-11U + t)^2 - 4(30U^2 - 6Ut - 2t^2)}}{2}, \quad (66f)
$$

and the eigenvalues below half filling are

$$
\lambda_{A_{11}}^{N_e=2,S_z=0} = \frac{5U - 2t + \sqrt{(-5U + 2t)^2 - 4(6U^2 - 6Ut - 8t^2)}}{2}, \quad (67a)
$$

$$
\lambda_{A_{12}}^{N_e=2,S_z=0} = \frac{5U - 2t - \sqrt{(-5U + 2t)^2 - 4(6U^2 - 6Ut - 8t^2)}}{2}, \quad (67b)
$$

$$
\lambda_{A_2}^{N_e=2,S_z=0} = 2U + 2t, \quad (67c)
$$

$$
\lambda_{E_1}^{N_e=2,S_z=0} = 2U - t, \quad (67d)
$$

$$
\lambda_{E_2}^{N_e=2,S_z=0} = \frac{5U + t + \sqrt{(-5U - t)^2 - 4(6U^2 + 3Ut - 2t^2)}}{2}, \quad (67e)
$$

$$
\lambda_{E_3}^{N_e=2,S_z=0} = \frac{5U + t - \sqrt{(-5U - t)^2 - 4(6U^2 + 3Ut - 2t^2)}}{2}. \quad (67f)
$$

Plots of the eigenvalues above (and below) half filling for $N_e = 4$ (and 2) and $S_z = 0$ are plotted in Fig. 8 (with the constant term of the Hubbard Hamiltonian, $4U$, subtracted off) showing the variation of the photoemission energies

This explains why $A_1$ and $A_{22}$ are degenerate for all $U$. Finally, we then can explain why the $E_3$ energy is lower than the $A_1$ and $A_{22}$ energy for finite $U$. This is because the $E_3$ state can have a component of Bloch state in panel (4) which is energetically lower for finite $U$ than in panel (3).
with $U$. The ground state energy of the half-filled system has been subtracted off of $\lambda^{N_e=4, S_z=0}$ and $\lambda^{N_e=2, S_z=0}$. Fig. 9 show the photoemission spectrum for different values of $U$.

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Appendix A: Triangular cluster solutions

Here we present the exact solutions to the Hubbard Hamiltonian for the triangular cluster in the following cases: half filling, $N_e = 3$, for $S_z = \frac{1}{2}$; above half filling, $N_e = 4$, for $S_z = 0, 1$; and, below half filling, $N_e = 4$, for $S_z = 0, 1$.

1. half filling: $N_e = 3$ and $S_z = \frac{1}{2}$

For $S_z = \frac{1}{2}$ in the case of half filling where $N_e = 3$ we have 9 elements in our basis. We choose our $\{\phi_n\}$ basis as follows:

$$
\phi_1 = |mpp\rangle \quad \phi_2 = |pmp\rangle \quad \phi_3 = |ppm\rangle \\
\phi_4 = |dpe\rangle \quad \phi_5 = |edp\rangle \quad \phi_6 = |ped\rangle \\
\phi_7 = |dep\rangle \quad \phi_8 = |pde\rangle \quad \phi_9 = |epd\rangle.
$$

(A1)
In the case of half filling, the \( \{ \psi_n \} \) basis states generated by the \( C_{3v} \) projection operators happen all to be eigenvectors of \( S^2 \), so here we do not get any reduction in block size using the total-spin. Therefore, the \( \{ \varphi_n \} \) basis is equivalent to \( \{ \psi_n \} \).
A TRIANGULAR CLUSTER SOLUTIONS

2 Above half filling: \( N_e = 4 \) and \( S_z = 0 \)

a. \( A_1 \) State with \( S = \frac{1}{2} \)

\[
\psi_1 = (\phi_4 + \phi_5 + \phi_6 + \phi_7 + \phi_8) / \sqrt{6} \rightarrow \langle H_{S=\frac{1}{2}}^{A_1} \rangle = (4U) . \tag{A2}
\]

b. \( A_2 \) States with \( S = \frac{1}{2}, \frac{3}{2} \)

\[
\psi_2 = (\phi_1 + \phi_2 + \phi_3) / \sqrt{3} \rightarrow \langle H_{S=\frac{3}{2}}^{A_2} \rangle = (3U) \tag{A3}
\]

\[
\psi_3 = (\phi_4 + \phi_5 + \phi_6 - \phi_7 - \phi_8) / \sqrt{6} \rightarrow \langle H_{S=\frac{1}{2}}^{A_2} \rangle = (4U) \tag{A4}
\]

c. \( E \) States with \( S = \frac{1}{2} \)

\[
\psi_4 = (\phi_1 + \epsilon \phi_2 + \epsilon^* \phi_3) / \sqrt{3} \rightarrow \langle H_{S=\frac{1}{2}}^{E} \rangle = \begin{pmatrix} 3U & (\epsilon^* - 1)t & (1 - \epsilon)t \\ (\epsilon - 1)t & 4U & (\epsilon^* - 1)t \\ (1 - \epsilon^*)t & (\epsilon - 1)t & 4U \end{pmatrix}, \tag{A5}
\]

where \( \epsilon = e^{-i \frac{2\pi}{3}} \).

2. Above half filling: \( N_e = 4 \) and \( S_z = 0 \)

For \( S_z = 0 \), above half filling where \( N_e = 4 \), we have 9 elements in our basis. We choose our \{\phi_n\} basis as follows

\[
\begin{align*}
\phi_1 & = |dmp \rangle \\
\phi_2 & = |pdm \rangle \\
\phi_3 & = |mpd \rangle \\
\phi_4 & = |dpm \rangle \\
\phi_5 & = |mdp \rangle \\
\phi_6 & = |pmd \rangle \\
\phi_7 & = |edd \rangle \\
\phi_8 & = |ded \rangle \\
\phi_9 & = |dde \rangle
\end{align*} \tag{A6}
\]

The \{\phi_n\} and \{\psi_n\} basis are equivalent in the \( A_1 \) and \( A_2 \) representations, for \( n = 1, 2, 3 \).

a. \( A_1 \) States with \( S = 0 \)

\[
\varphi_1 = \psi_1 = (\phi_1 - \phi_2 + \phi_3 - \phi_4 + \phi_5 - \phi_6) / \sqrt{6} \rightarrow \langle H_{S=0}^{A_1} \rangle = \begin{pmatrix} 5U + 2t & 4t \sqrt{2} \\ 4t \sqrt{2} & 6U \end{pmatrix}. \tag{A7}
\]

b. \( A_2 \) State with \( S = 1 \)

\[
\varphi_3 = \psi_3 = (\phi_1 - \phi_2 + \phi_3 + \phi_4 - \phi_5 + \phi_6) / \sqrt{6} \rightarrow \langle H_{S=1}^{A_2} \rangle = (5U - 2t) . \tag{A8}
\]
c. E States with $S = 0, 1$

\[
\psi_4 = \frac{(2\phi_1 + \phi_2 - \phi_3)}{\sqrt{5}} \quad \text{(A9a)} \\
\psi_5 = \frac{(2\phi_4 + \phi_5 - \phi_6)}{\sqrt{5}} \quad \text{(A9b)} \\
\psi_6 = \frac{(2\phi_7 - \phi_8 - \phi_9)}{\sqrt{5}} \quad \text{(A9c)}
\]

\[
\varphi_4 = \frac{(\psi_4 + \psi_5)}{\sqrt{2}} \rightarrow \langle H^{E}_{S=1} \rangle = (5U + t) \quad \text{(A10)}
\]

\[
\varphi_5 = \frac{(\psi_4 - \psi_5)}{\sqrt{2}} \rightarrow \langle H^{E}_{S=0} \rangle = \left(\frac{5U - \frac{2t}{\sqrt{2}}}{6U}\right) \quad \text{(A11)}
\]

3. Above half filling: $N_e = 4$ and $S_z = 1$

For $S_z = 1$, above half filling where $N_e = 4$, we have 3 elements in our basis. We choose our $\{\phi_n\}$ basis as follows

\[
\phi_1 = |dpp\rangle \quad \phi_2 = |pdp\rangle \quad \phi_3 = |ppd\rangle \quad \phi_4 = |emp\rangle \quad \phi_5 = |pem\rangle \quad \phi_6 = |mpe\rangle \quad \phi_7 = |dee\rangle \quad \phi_8 = |ede\rangle \quad \phi_9 = |eed\rangle
\]

(a) $A_2$ State with $S = 1$

\[
\varphi_1 = \psi_1 = (\phi_1 - \phi_2 + \phi_3)/\sqrt{3} \rightarrow \langle H^{A_2}_{S=1} \rangle = (5U - 2t) \quad \text{(A13)}
\]

(b) $E$ State with $S = 1$

\[
\varphi_2 = \psi_2 = (2\phi_1 + \phi_2 - \phi_3)/\sqrt{3} \rightarrow \langle H^{E}_{S=1} \rangle = (5U + t) \quad \text{(A14)}
\]

4. Below half filling: $N_e = 2$ and $S_z = 0$

For $S_z = 0$, below half filling where $N_e = 2$, we have 9 elements in our basis. We choose our $\{\phi_n\}$ basis as follows

\[
\phi_1 = |emp\rangle \quad \phi_2 = |pem\rangle \quad \phi_3 = |mpe\rangle \quad \phi_4 = |epm\rangle \quad \phi_5 = |mep\rangle \quad \phi_6 = |pme\rangle \quad \phi_7 = |dee\rangle \quad \phi_8 = |ede\rangle \quad \phi_9 = |eed\rangle
\]

The $\{\varphi_n\}$ and $\{\psi_n\}$ basis are equivalent in the $A_1$ and $A_2$ representations, for $n = 1, 2, 3$.

(a) $A_1$ States with $S = 0$

\[
\varphi_1 = \psi_1 = (\phi_1 - \phi_2 + \phi_3 - \phi_4 + \phi_5)/\sqrt{6} \rightarrow \langle H^{A_1}_{S=0} \rangle = \begin{pmatrix} 2U - 2t & 2\sqrt{2}t \\ 2\sqrt{2}t & 3U \end{pmatrix} \quad \text{(A16)}
\]
b. $A_2$ State with $S = 1$

$$\varphi_3 = \psi_3 = (\phi_1 - \phi_2 + \phi_3 + \phi_4 - \phi_5 + \phi_6)/\sqrt{6} \rightarrow \langle H_{S=1}^{A_2} \rangle = (2U + 2t). \quad (A17)$$

c. $E$ States with $S = 0, 1$

$$\psi_4 = (2\phi_1 + \phi_2 - \phi_3)/\sqrt{5} \quad (A18a)$$
$$\psi_5 = (2\phi_4 + \phi_5 - \phi_6)/\sqrt{5} \quad (A18b)$$
$$\psi_6 = (2\phi_7 - \phi_8 - \phi_9)/\sqrt{5} \quad (A18c)$$

$$\varphi_4 = (\psi_4 + \psi_5)/\sqrt{2} \rightarrow \langle H_{S=1}^{E} \rangle = (2U - t) \quad (A19)$$

$$\varphi_5 = (\psi_4 - \psi_5)/\sqrt{2} \rightarrow \langle H_{S=0}^{E} \rangle = \left(2U + t \frac{-2t}{\sqrt{2}} \frac{2t}{\sqrt{2}} \frac{3U}{\sqrt{2}} \right). \quad (A20)$$

5. Below half filling: $N_e = 2$ and $S_z = 1$

For $S_z = 1$, below half filling where $N_e = 2$, we have 3 elements in our basis. We choose our $\{\phi_n\}$ basis as follows

$$\phi_1 = |epp\rangle \quad \phi_2 = |pep\rangle \quad \phi_3 = |ppe\rangle. \quad (A21)$$

The $\{\phi_n\}$ and $\{\psi_n\}$ basis are equivalent. There are no states in the $A_1$ representation.

a. $A_2$ State with $S = 1$

$$\varphi_1 = \psi_1 = (\phi_1 - \phi_2 + \phi_3)/\sqrt{3} \rightarrow \langle H_{S=1}^{A_2} \rangle = (2U + 2t). \quad (A22)$$

b. $E$ State with $S = 1$

$$\varphi_2 = \psi_2 = (2\phi_1 + \phi_2 - \phi_3)/\sqrt{5} \rightarrow \langle H_{S=1}^{E} \rangle = (2U - t). \quad (A23)$$

Appendix B: Square cluster solutions

In this section we present our findings for the square cluster for the case of half filling, $N_e = 4$, for $S_z = 0$. 

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1. Half filling: \( N_e = 4 \) and \( S_z = 0 \)

For \( S_z = 0 \) in the case of half filling where \( N_e = 4 \) we have 36 elements in our basis. We choose our \( \{ \phi_n \} \) basis as follows

\[
\begin{align*}
\phi_1 &= |mpmp\rangle & \phi_2 &= |mpmp\rangle \\
\phi_3 &= |ppmm\rangle & \phi_4 &= |mpmm\rangle & \phi_5 &= |mmpp\rangle & \phi_6 &= |pnmn\rangle \\
\phi_7 &= |demp\rangle & \phi_8 &= |pedm\rangle & \phi_9 &= |mpdc\rangle & \phi_{10} &= |empd\rangle \\
\phi_{11} &= |dpme\rangle & \phi_{12} &= |edpm\rangle & \phi_{13} &= |medp\rangle & \phi_{14} &= |pmde\rangle \\
\phi_{15} &= |depm\rangle & \phi_{16} &= |mdep\rangle & \phi_{17} &= |pmde\rangle & \phi_{18} &= |empd\rangle \\
\phi_{19} &= |dmpe\rangle & \phi_{20} &= |edmp\rangle & \phi_{21} &= |pedm\rangle & \phi_{22} &= |mpde\rangle \\
\phi_{23} &= |dmep\rangle & \phi_{24} &= |pdme\rangle & \phi_{25} &= |epdm\rangle & \phi_{26} &= |mepd\rangle \\
\phi_{27} &= |dpem\rangle & \phi_{28} &= |mdpe\rangle & \phi_{29} &= |emdp\rangle & \phi_{30} &= |pmded\rangle \\
\phi_{31} &= |ddee\rangle & \phi_{32} &= |edde\rangle & \phi_{33} &= |edde\rangle & \phi_{34} &= |edde\rangle & \phi_{35} &= |edde\rangle & \phi_{36} &= |edde\rangle \
\end{align*}
\]  

\( (B1) \)

a. \( A_1 \) States with \( S = 0, 1 \)

\[
\begin{align*}
\psi_1 &= (\phi_3 - \phi_4 + \phi_5 - \phi_6)/2 \\
\psi_2 &= (\phi_7 - \phi_8 + \phi_9 - \phi_{10} + \phi_{11} - \phi_{12} + \phi_{13} - \phi_{14})/\sqrt{8} \\
\psi_3 &= (\phi_{15} - \phi_{16} + \phi_{17} + \phi_{18} + \phi_{19} - \phi_{20} - \phi_{21} + \phi_{22})/\sqrt{8} \\
\psi_4 &= (\phi_{23} - \phi_{24} - \phi_{25} + \phi_{26} - \phi_{27} + \phi_{28} + \phi_{29} - \phi_{30})/\sqrt{8} \\
\psi_5 &= (\phi_{31} + \phi_{32})/\sqrt{2} \\
\psi_6 &= (\phi_{33} + \phi_{34} + \phi_{35} + \phi_{36})/2 \\
\end{align*}
\]  

\( (B2a) \)

\[
\begin{align*}
\varphi_1 &= (\psi_2 + \psi_3)/\sqrt{2} \rightarrow \langle H_{S=1}^{A_1} \rangle = (5U). \\
\varphi_2 &= \psi_4 \\
\varphi_3 &= \psi_1 \\
\varphi_4 &= (\psi_2 - \psi_3)/\sqrt{2} \rightarrow \langle H_{S=0}^{A_1} \rangle = \begin{pmatrix} 5U & 0 & 0 & 0 \\
0 & 4\sqrt{2} & 2t & 0 \\
0 & 2U & 5U & \frac{4t}{\sqrt{2}} \\
0 & 0 & \frac{4t}{\sqrt{2}} & 6U & 0 \\
0 & 0 & 2t & 0 & 6U \end{pmatrix}. \\
\varphi_5 &= \psi_5 \\
\varphi_6 &= \psi_6 \\
\end{align*}
\]  

\( (B3) \)

b. \( A_2 \) States with \( S = 0, 1 \)

\[
\begin{align*}
\psi_7 &= (\phi_1 - \phi_2)/\sqrt{2} \\
\psi_8 &= (\phi_7 - \phi_8 + \phi_9 + \phi_{10} + \phi_{11} + \phi_{12} + \phi_{13} + \phi_{14})/\sqrt{8} \\
\psi_9 &= (\phi_{15} - \phi_{16} + \phi_{17} + \phi_{18} + \phi_{19} - \phi_{20} + \phi_{21} - \phi_{22})/\sqrt{8} \\
\psi_{10} &= (\phi_{23} - \phi_{24} - \phi_{25} + \phi_{26} - \phi_{27} + \phi_{28} - \phi_{29} + \phi_{30})/\sqrt{8} \\
\end{align*}
\]  

\( (B5a) \)

\[
\begin{align*}
\varphi_7 &= \psi_7 \\
\varphi_8 &= \psi_{10} \\
\varphi_9 &= (\psi_8 + \psi_9)/\sqrt{2} \rightarrow \langle H_{S=1}^{A_2} \rangle = \begin{pmatrix} 4U & 0 & 0 & 0 \\
0 & \frac{4t}{\sqrt{2}} & 0 & 0 \\
0 & 5U & \frac{4t}{\sqrt{2}} & 2t \\
\frac{4t}{\sqrt{2}} & -\frac{4t}{\sqrt{2}} & 5U & 0 \end{pmatrix}. \\
\varphi_{10} &= (\psi_8 - \psi_9)/\sqrt{2} \rightarrow \langle H_{S=0}^{A_2} \rangle = (5U). \\
\end{align*}
\]  

\( (B7) \)
Half filling: $N_z = 4$ and $S_z = 0$

**B SQUARE CLUSTER SOLUTIONS**

c. $B_1$ States with $S = 0, 1$

$$\psi_{11} = (\phi_7 + \phi_8 + \phi_9 - \phi_{10} - \phi_{11} + \phi_{12} + \phi_{13} + \phi_{14})/\sqrt{8} \quad (B8a)$$
$$\psi_{12} = (\phi_{15} + \phi_{16} + \phi_{17} - \phi_{18} - \phi_{19} + \phi_{20} + \phi_{21} + \phi_{22})/\sqrt{8} \quad (B8b)$$
$$\psi_{13} = (\phi_{23} + \phi_{24} - \phi_{25} - \phi_{26} - \phi_{27} - \phi_{28} + \phi_{29} + \phi_{30})/\sqrt{8} \quad (B8c)$$
$$\psi_{14} = (\phi_{31} - \phi_{32})/\sqrt{2} \quad (B8d)$$

$$\varphi_{11} = (\psi_{11} + \psi_{12})/\sqrt{2} \rightarrow \langle H_{S=1}^{B_1} \rangle = (5U). \quad (B9)$$

$$\begin{aligned} 
\varphi_{12} &= (\psi_{11} - \psi_{12})/\sqrt{2} \\
\varphi_{13} &= \psi_{13} \\
\varphi_{14} &= \psi_{14}
\end{aligned} \rightarrow \langle H_{S=0}^{B_1} \rangle = \begin{pmatrix} 5U & -\frac{4t}{\sqrt{2}} & \frac{4t}{\sqrt{2}} \\ -\frac{4t}{\sqrt{2}} & 5U & 0 \\ 0 & 0 & 6U \end{pmatrix}. \quad (B10)$$

d. $B_2$ States with $S = 0, 1, 2$

$$\psi_{15} = (\phi_1 + \phi_2)/\sqrt{2} \quad (B11a)$$
$$\psi_{16} = (\phi_3 + \phi_4 + \phi_5 + \phi_6)/2 \quad (B11b)$$
$$\psi_{17} = (\phi_7 + \phi_8 + \phi_9 - \phi_{10} - \phi_{11} - \phi_{12} - \phi_{13} - \phi_{14})/\sqrt{8} \quad (B11c)$$
$$\psi_{18} = (\phi_{15} + \phi_{16} + \phi_{17} - \phi_{18} + \phi_{19} - \phi_{20} - \phi_{21} - \phi_{22})/\sqrt{8} \quad (B11d)$$
$$\psi_{19} = (\phi_{23} + \phi_{24} - \phi_{25} - \phi_{26} + \phi_{27} + \phi_{28} - \phi_{29} + \phi_{30})/\sqrt{8} \quad (B11e)$$
$$\psi_{20} = (\phi_{33} - \phi_{34} - \phi_{35} + \phi_{36})/\sqrt{4} \quad (B11f)$$

$$\varphi_{15} = (\psi_{15}/\sqrt{2} + \psi_{16})/\sqrt{3/2} \rightarrow \langle H_{S=2}^{B_2} \rangle = (4U). \quad (B12)$$

$$\begin{aligned} 
\varphi_{16} &= (\psi_{17} + \psi_{18})/\sqrt{2} \\
\varphi_{17} &= \psi_{19}
\end{aligned} \rightarrow \langle H_{S=1}^{B_2} \rangle = \begin{pmatrix} 5U & 0 \\ 0 & 5U \end{pmatrix}. \quad (B13)$$

$$\begin{aligned} 
\varphi_{18} &= (-2\psi_{15}/\sqrt{2} + \psi_{16})/\sqrt{3} \\
\varphi_{19} &= (\psi_{17} - \psi_{18})/\sqrt{2} \\
\varphi_{20} &= \psi_{20}
\end{aligned} \rightarrow \langle H_{S=0}^{B_2} \rangle = \begin{pmatrix} 4U & -\frac{6t}{\sqrt{3}} & 0 \\ -\frac{6t}{\sqrt{3}} & 5U & -2t \\ 0 & -2t & 6U \end{pmatrix}. \quad (B14)$$

Although $\varphi_{16}$ and $\varphi_{17}$ have the same total-spin, not that they happen to be eigenvectors the Hamiltonian.

e. $E$ States with $S = 0, 1$

$$\psi_{21} = (\phi_3 - i\phi_4 - \phi_5 + i\phi_6)/2 \quad (B15a)$$
$$\psi_{22} = (\phi_7 - i\phi_8 - \phi_9 - i\phi_{10})/2 \quad (B15b)$$
$$\psi_{23} = (\phi_{11} + i\phi_{12} + \phi_{13} - i\phi_{14})/2 \quad (B15c)$$
$$\psi_{24} = (\phi_{15} - i\phi_{16} + \phi_{17} - i\phi_{18})/2 \quad (B15d)$$
$$\psi_{25} = (\phi_{19} + i\phi_{20} + \phi_{21} - i\phi_{22})/2 \quad (B15e)$$
$$\psi_{26} = (\phi_{23} - i\phi_{24} + \phi_{25} - i\phi_{26})/2 \quad (B15f)$$
$$\psi_{27} = (\phi_{27} - i\phi_{28} + \phi_{29} - i\phi_{30})/2 \quad (B15g)$$
$$\psi_{28} = (\phi_{33} - i\phi_{34} + \phi_{35} - i\phi_{36})/2 \quad (B15h)$$
\[ \begin{align*}
\varphi_{21} &= \psi_{21} \\
\varphi_{22} &= (\psi_{26} + \psi_{27})/\sqrt{2} \\
\varphi_{23} &= (\psi_{23} + \psi_{25})/\sqrt{2} \\
\varphi_{24} &= (\psi_{22} + \psi_{24})/\sqrt{2}
\end{align*} \]

\[ \rightarrow \langle H_{S=1}^E \rangle = \begin{pmatrix} 4U & 0 & -2t \sqrt{2} \\ 0 & 5U & (1 + i) t \\ -2t \sqrt{2} & 5U & 0 \end{pmatrix}. \quad (B16) \]

\[ \begin{align*}
\varphi_{25} &= (\psi_{23} + \psi_{25})/\sqrt{2} \\
\varphi_{26} &= (\psi_{22} + \psi_{24})/\sqrt{2} \\
\varphi_{27} &= (\psi_{26} - \psi_{27})/\sqrt{2} \\
\varphi_{28} &= \psi_{28}
\end{align*} \]

\[ \rightarrow \langle H_{S=0}^E \rangle = \begin{pmatrix} 5U & 0 & (-1 + i) t \sqrt{2} \\ 0 & 5U & (1 + i) t \sqrt{2} \\ (-1 - i) t & (1 - i) t & 5U & 0 \end{pmatrix}. \quad (B17) \]

References

Cotton, F., 1964, Chemical applications of group theory.