HUBBARD MODEL OF A SOLID

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The simplified Hubbard model of a solid (described in Lancaster & Blundell's Chapter 4) proposes that the Hamiltonian is

$$H = \sum_{ij\sigma} (-t_{ij})\, c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} \tag{1}$$

In this model, the solid is represented by a lattice with each location in the lattice indexed by a Roman letter (i, j). Each lattice site can be occupied by zero or more electrons (provided that that the electrons obey the Pauli exclusion principle if they occupy the same site). The spin of an electron is represented by σ.

The model is a form of tight-binding. It's assumed that when an electron hops between sites i and j, its kinetic energy is reduced by an amount $-t_{ij}$. The potential energy U is due to the Coulomb interaction and is assumed to be significant only when two electrons occupy the same lattice site i. In this case, the spins of the two electrons must be opposite to satisfy the exclusion principle.

The kinetic energy term consists of an annihilation operator $c_{j\sigma}$ which annihilates an electron at site j and a creation operator $c^{\dagger}_{j\sigma}$ which creates an electron at site i. The spin σ of the electron is assumed not to change during the hop from one site to another. Since $-t_{ij}$ represents the kinetic energy reduction in hopping from one site to another, $t_{ii} = 0$ since there is no change in the kinetic energy if the electron stays at the same site.

In the potential energy term, U is the Coulomb energy between the electrons at the same site. The operator $n_{i\sigma}$ is the number operator ($n_{i\sigma} = c^{\dagger}_{i\sigma} c_{i\sigma}$) which counts the number of electrons with spin σ at site i. There must be at least 2 electrons at a site in order for this term to be non-zero.

In L&B's example 4.11, they consider a simple model with two sites and either one or two electrons. In the one-electron case, the potential energy term is zero, and the single electron can only hop between the two sites. We represent the state of the system by the ket $|\uparrow, 0\rangle$ if the electron has spin up and occupies site 1 and by $|0, \uparrow\rangle$ for a spin-up electron on site 2. We take the

kinetic energy saving to be $-t$ for both possible hops. The matrix elements of H are then

$$H = \begin{bmatrix} 0 & -t \\ -t & 0 \end{bmatrix} \tag{2}$$

where the top row and first column represent $|\uparrow, 0\rangle$ and the bottom row and second column represent $|0, \uparrow\rangle$. For example

$$\langle \uparrow, 0 | H | 0, \uparrow \rangle = \left\langle \uparrow, 0 \left| \sum_{ij\sigma} (-t_{ij})\, c_{i\sigma}^{\dagger} c_{j\sigma} \right| 0, \uparrow \right\rangle \tag{3}$$

$$= -\left\langle \uparrow, 0 \left| t c_{1\uparrow}^{\dagger} c_{2\uparrow} \right| 0, \uparrow \right\rangle \tag{4}$$

$$= -t \tag{5}$$

where the second line follows because all other terms in the sum from the first line are zero, as they involve an annihilation operator $c_{j\sigma}$ which annihilates a state that is not $|0, \uparrow\rangle$.

The eigenvalues of 2 are $-t$ eigenvector $|\uparrow, 0\rangle + |0, \uparrow\rangle$ (the ground state) and $+t$ with eigenvector $|\uparrow, 0\rangle - |0, \uparrow\rangle$ (the excited state).

With two electrons, the possible states are

$$|\uparrow\downarrow, 0\rangle\,,\ |\uparrow, \downarrow\rangle\,,\ |\downarrow, \uparrow\rangle\,,\ |0, \uparrow\downarrow\rangle \tag{6}$$

As the model allows only a single electron hop at a time, transitions are possible only between the state $|\uparrow\downarrow, 0\rangle$ and $|\uparrow, \downarrow\rangle$ or $|\downarrow, \uparrow\rangle$, or between $|0, \uparrow\downarrow\rangle$ and $|\uparrow, \downarrow\rangle$ or $|\downarrow, \uparrow\rangle$. Transitions between any other pair of states involves hopping two electrons at once. For example, to hop between $|\uparrow, \downarrow\rangle$ and $|\downarrow, \uparrow\rangle$, we'd need to hop the spin-up electron from site 1 to 2 and the spin-down electron from site 2 to 1.

Only the states $|\uparrow\downarrow, 0\rangle$ and $|0, \uparrow\downarrow\rangle$ have any potential energy, since they are the only states where two electrons occupy the same site. The matrix elements of H are now

$$H = \begin{bmatrix} U & -t & -t & 0 \\ -t & 0 & 0 & -t \\ -t & 0 & 0 & -t \\ 0 & -t & -t & U \end{bmatrix} \tag{7}$$

We can find the eigenvalues and eigenvectors of this matrix (by hand, if you want to go through the slog, or using Maple, as I did), and we get eigenvalues of

$$E = U,\ \frac{U}{2} + \frac{\sqrt{U^2+16t^2}}{2},\ \frac{U}{2} - \frac{\sqrt{U^2+16t^2}}{2},\ 0 \tag{8}$$

Since $U > 0$, the ground state is $\frac{U}{2} - \frac{\sqrt{U^2+16t^2}}{2} < 0$ and the excited states are 0, U and $\frac{U}{2} + \frac{\sqrt{U^2+16t^2}}{2}$, in ascending order.

Maple gives for the eigenvectors:

- Eigenvalue $\frac{U}{2} - \frac{\sqrt{U^2+16t^2}}{2}$:

$$\begin{bmatrix} 1 \\ \frac{4t}{-U+\sqrt{U^2+16t^2}} \\ \frac{4t}{-U+\sqrt{U^2+16t^2}} \\ 1 \end{bmatrix} \tag{9}$$

We can convert this into the answer given in L&B by multiplying the middle two elements by

$$\frac{U+\sqrt{U^2+16t^2}}{U+\sqrt{U^2+16t^2}} \tag{10}$$

from which we get

$$|\psi_0\rangle = N\left(|\uparrow\downarrow,0\rangle + W|\uparrow,\downarrow\rangle + W|\downarrow,\uparrow\rangle + |0,\uparrow\downarrow\rangle\right) \tag{11}$$

with N a normalization constant and

$$W \equiv \frac{1}{4t}\left(U + \sqrt{U^2+16t^2}\right) \tag{12}$$

The other states are

- Eigenvalue 0:

$$|\psi_1\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle\right) \tag{13}$$

- Eigenvalue U:

$$|\psi_2\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow,0\rangle - |0,\uparrow\downarrow\rangle\right) \tag{14}$$

- Eigenvalue $\frac{U}{2} + \frac{\sqrt{U^2+16t^2}}{2}$:

$$|\psi_3\rangle = N\left(|\uparrow\downarrow,0\rangle - \frac{4t}{U+\sqrt{U^2+16t^2}}|\uparrow,\downarrow\rangle - \frac{4t}{U+\sqrt{U^2+16t^2}}|\downarrow,\uparrow\rangle + |0,\uparrow\downarrow\rangle\right) \tag{15}$$

$$= N\left(|\uparrow\downarrow,0\rangle + Y|\uparrow,\downarrow\rangle + Y|\downarrow,\uparrow\rangle + |0,\uparrow\downarrow\rangle\right) \tag{16}$$

with

$$Y \equiv \frac{1}{4t}\left(U - \sqrt{U^2 + 16t^2}\right) \tag{17}$$

In the limit $t \to 0$ (so there is no kinetic energy gain from hopping sites), we note that, as $t \to 0$:

$$W = \frac{1}{4t}\left(U + \sqrt{U^2 + 16t^2}\right) \tag{18}$$

$$= \frac{U}{4t}\left(1 + \sqrt{1 + \left(\frac{4t}{U}\right)^2}\right) \tag{19}$$

$$\to \frac{U}{4t}\left(2 + 8\frac{t^2}{U^2} + \ldots\right) \tag{20}$$

$$\to \infty \tag{21}$$

Also

$$Y = \frac{1}{4t}\left(U - \sqrt{U^2 + 16t^2}\right) \tag{22}$$

$$= \frac{U}{4t}\left(1 - \sqrt{1 + \left(\frac{4t}{U}\right)^2}\right) \tag{23}$$

$$\to \frac{U}{4t}\left(-8\frac{t^2}{U^2} + \ldots\right) \tag{24}$$

$$\to 0 \tag{25}$$

The energies have the limits $E_0 \to 0$, $E_1 = 1$, $E_2 = U$ and $E_3 \to U$, so we get

$$|\psi_0\rangle \to \frac{1}{\sqrt{2}}\left(|\uparrow,\downarrow\rangle + |\downarrow,\uparrow\rangle\right); \quad E_0 \to 0 \tag{26}$$

$$|\psi_1\rangle \to \frac{1}{\sqrt{2}}\left(|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle\right); \quad E_1 \to 0 \tag{27}$$

$$|\psi_2\rangle \to \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow,0\rangle - |0,\uparrow\downarrow\rangle\right); \quad E_2 \to U \tag{28}$$

$$|\psi_3\rangle \to \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow,0\rangle + |0,\uparrow\downarrow\rangle\right); \quad E_3 \to U \tag{29}$$

Thus there are two degenerate energies rather than the four we started with.

As t increases from zero, we can examine the behaviour of the energies for $\tau \equiv \frac{t}{U} \ll 1$. The ground state is

$$E_0 = \frac{U}{2} - \frac{\sqrt{U^2+16t^2}}{2} \tag{30}$$

$$= \frac{U}{2}\left(1-\sqrt{1+16\tau^2}\right) \tag{31}$$

$$= \frac{U}{2}\left(-8\tau^2+\mathcal{O}\left(\tau^4\right)\right) \tag{32}$$

Thus for small t, we have

$$E_0 \approx -4\frac{t^2}{U} \tag{33}$$

Similarly, for E_3 we have

$$E_3 = \frac{U}{2} + \frac{\sqrt{U^2+16t^2}}{2} \tag{34}$$

$$= \frac{U}{2}\left(1+\sqrt{1+16\tau^2}\right) \tag{35}$$

$$= \frac{U}{2}\left(8\tau^2+\mathcal{O}\left(\tau^4\right)\right) \tag{36}$$

$$\approx +4\frac{t^2}{U} \tag{37}$$