Second quantization - additional examples

In these notes we continue to explore the physics of Hamiltonians written in the language of 2nd quantization. To begin, let us explore a bit more the double well problem for Bosons. In particular, I want to look at it from a dynamical point of view.

The Hamiltonian is

$$H = \sum_{i=L,R} \left\{ \epsilon a_i^\dagger a_i + \frac{U}{2} a_i^\dagger a_i (a_i^\dagger a_i - 1) \right\} + J (a_L^\dagger a_R + a_R^\dagger a_L) \tag{1}$$

And what I want to do is solve Schrödinger's equation

$$i \partial_t |\psi\rangle = H |\psi\rangle \tag{2}$$

We can expand $|\psi\rangle$ in the Fock basis

$$|\psi_t\rangle = \sum_{N_L, N_R = 0}^{\infty} \psi_t(N_L, N_R) \, |N_L, N_R\rangle \tag{3}$$

But a state like this is a superposition of states with different numbers of particles, which seems a bit strange. Instead, it is more natural to have a situation where the number of particles is well defined. This is where particle conservation comes in. If we start with N particles at t=0, we will continue to have N particles for all further times.

So, for instance, let us assume that we have only $N=2$ particles. Then there are only 3 Fock states : $|2,0\rangle$, $|1,1\rangle$, $|0,2\rangle$.

Thus, any $|\psi_t\rangle$ may be parametrized as

$$|\psi_t\rangle = \psi_+(t)\,|2,0\rangle + \psi_0(t)\,|1,1\rangle + \psi_-(t)\,|0,2\rangle \tag{4}$$

where, for simplicity, I'm writing $\psi_+ = \psi(2,0)$ and so on.

Now let's see how H in Eq (1) acts on these 3 Fock states.

Note that

$$\begin{aligned}
(a_L^\dagger a_R + a_R^\dagger a_L)\,|2,0\rangle &= \sqrt{2}\,|1,1\rangle \\
(a_L^\dagger a_R + a_R^\dagger a_L)\,|1,1\rangle &= \sqrt{2}\,|2,0\rangle + \sqrt{2}\,|0,2\rangle \\
(a_L^\dagger a_R + a_R^\dagger a_L)\,|0,2\rangle &= \sqrt{2}\,|1,1\rangle
\end{aligned} \tag{5}$$

Thus

$$H|2,0\rangle = (2\epsilon + U)\,|2,0\rangle + \sqrt{2}\,J\,|1,1\rangle \tag{6a}$$

$$H|1,1\rangle = 2\epsilon\,|1,1\rangle + \sqrt{2}\,J\,|2,0\rangle + \sqrt{2}\,J\,|0,2\rangle \tag{6b}$$

$$H|0,2\rangle = (2\epsilon + U)\,|0,2\rangle + \sqrt{2}\,J\,|1,1\rangle \tag{6c}$$

From this we can reconstruct the Hamiltonian matrix in the $N=2$ subspace. For instance, from (6a) we find that

$$\langle 2,0|H|2,0\rangle = 2\epsilon + U$$

$$\langle 1,1|H|2,0\rangle = \sqrt{2}\,J$$

$$\langle 0,2|H|2,0\rangle = 0$$

This represents the first column of the matrix.

We then get

$$H_2 = \begin{pmatrix} 2\epsilon + U & \sqrt{2}\,J & 0 \\ \sqrt{2}\,J & 2\epsilon & \sqrt{2}\,J \\ 0 & \sqrt{2}\,J & 2\epsilon + U \end{pmatrix} \tag{7}$$

within this $N=2$ subspace, the state (4) will thus evolve according to

$$i\frac{d}{dt}\begin{pmatrix} \psi_+ \\ \psi_0 \\ \psi_- \end{pmatrix} = H_2 \begin{pmatrix} \psi_+ \\ \psi_0 \\ \psi_- \end{pmatrix} \tag{8}$$

the important conclusion that I want you to take from this is that if we start in the subspace $\{|2,0\rangle, |1,1\rangle, |0,2\rangle\}$ we continue in this subspace throughout.

From now on I will set $\epsilon = 0$ in Eq (7), since energy is defined only up to a constant. I will also, for simplicity, define

$$\alpha = 4J \tag{9}$$

Then (7) becomes

$$H_2 = \begin{pmatrix} U & \alpha/2\sqrt{2} & 0 \\ \alpha/2\sqrt{2} & 0 & \alpha/2\sqrt{2} \\ 0 & \alpha/2\sqrt{2} & U \end{pmatrix} \tag{10}$$

The eigenvalues of H_2 are then

$$\lambda_+ = \frac{1}{2}\left(U + \sqrt{U^2 + x^2}\right) \tag{11a}$$

$$\lambda_0 = U \tag{11b}$$

$$\lambda_- = \frac{1}{2}\left(U - \sqrt{U^2 + x^2}\right) \tag{11c}$$

the ground-state is always λ_-.

As for the matrix of eigenvectors, with some fooling around Mathematica one may show that we can write

$$S = \begin{pmatrix} -\frac{\cos\theta}{\sqrt{2}} & 1/\sqrt{2} & \frac{\sin\theta}{\sqrt{2}} \\ \sin\theta & 0 & \cos\theta \\ -\frac{\cos\theta}{\sqrt{2}} & -1/\sqrt{2} & \frac{\sin\theta}{\sqrt{2}} \end{pmatrix} \tag{12}$$

where

$$\tan(2\theta) = -\frac{x}{U} \tag{13}$$

We then get

$$H_2 = S \Lambda S^t \tag{14}$$

$$\Lambda = \mathrm{diag}(\lambda_+, \lambda_0, \lambda_-)$$

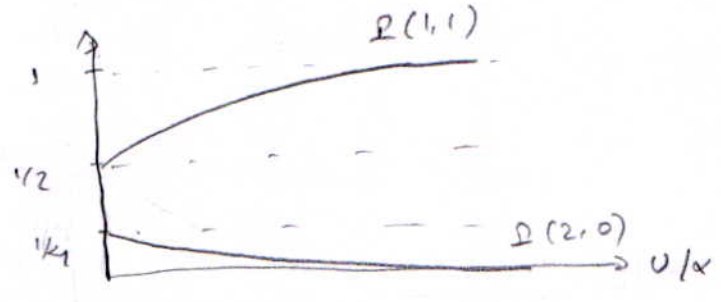
It is interesting to analyze these eigenvectors. In particular the ground state λ_-. The corresponding eigenvector is

$$\vec{v}_- = \begin{pmatrix} \sin\theta/\sqrt{2} \\ \cos\theta \\ \sin\theta/\sqrt{2} \end{pmatrix} \tag{15}$$

We can then analyze the probabilities of finding the system in $|2,0\rangle$, $|1,1\rangle$, $|0,2\rangle$, given it is in the GS:

$$P(2,0) = P(0,2) = \frac{\sin^2\theta}{2} \qquad P(1,1) = \cos^2\theta \tag{16}$$

If we plot these guys as a function of U/κ, we get



Remember that U has the tendency of localizing the wavefunction. If $U = 0$ we see that $P(2,0) = 1/4$ and $P(1,1) = 1/2$. The state is highly delocalized. Conversely, as U becomes large, $P(1,1)$ becomes dominant. Large U penalizes tunneling, forcing the particles to stay each in its own site.

Finally, we can study the dynamics of Eq (8). We simply need to write

$$e^{-iH_2 t} = S\, e^{-i\Lambda t}\, S^{\dagger} \tag{17}$$

For instance, suppose that at $t=0$ the system was prepared on $|1,1\rangle$. That is

$$|\psi_0\rangle = |1,1\rangle.$$

then at time t we will have

$$\psi_+(t) = \psi_-(t) = \frac{\sin 2\theta}{2\sqrt{2}}\left(e^{-i\lambda_- t} - e^{-i\lambda_+ t}\right) \tag{18}$$

$$\psi_0(t) = e^{-i\lambda_- t}\cos^2\theta + e^{-i\lambda_+ t}\sin^2\theta \tag{19}$$

Let

$$\Omega = \frac{1}{2}\sqrt{v^2 + \alpha^2}$$

Then

$$\psi_{\pm}(t) = \frac{\sin 2\theta}{2\sqrt{2}}\, e^{-iUt}\left(e^{i\Omega t} - e^{-i\Omega t}\right)$$

$$= \frac{e^{-iUt}}{\sqrt{2}}\,\frac{(-v)}{\sqrt{v^2+\alpha^2}}\, i \sin\Omega t$$

Thus, the probabilities becomes

$$|\psi_\pm|^2 = \frac{1}{2}\frac{\alpha^2}{U^2+\alpha^2}\sin^2\Omega t \tag{20}$$

Sanity check: if $\alpha = 0$ we get $\psi_\pm = 0$ because then there can be no tunneling.

We can also do another cool thing, which is to look at the reduced density matrix of the left site. Yes, everything we learned about density matrices, entanglement, and so on, continues to hold in this case.

So, we start with a general state like (4) and compute.

$$\rho = |\psi\rangle\langle\psi| = |\psi_+|^2 |2,0\rangle\langle 2,0| + \psi_+\psi_0^* |2,0\rangle\langle 1,1| + \psi_+\psi_-^* |2,0\rangle\langle 0,2|$$
$$+ \psi_0\psi_+^* |1,1\rangle\langle 2,0| + |\psi_0|^2 |1,1\rangle\langle 1,1| + \psi_0\psi_-^* |1,1\rangle\langle 0,2|$$
$$+ \psi_-\psi_+^* |0,2\rangle\langle 2,0| + \psi_-\psi_0^* |0,2\rangle\langle 2,0| + |\psi_-|^2 |0,2\rangle\langle 0,2|$$

Now we take the partial trace, for instance over R. We then get terms like

$$\mathrm{tr}_R |2,0\rangle\langle 2,0| = |2\rangle\langle 2| \,\mathrm{tr}\,(|0\rangle\langle 0|)$$
$$= |2\rangle\langle 2|$$

and

$$\mathrm{tr}_R |2,0\rangle\langle 1,1| = |2\rangle\langle 1| \,\mathrm{tr}\,(|0\rangle\langle 1|)$$
$$= 0$$

Thus

$$\rho_L = |\psi_+|^2 |2\rangle\langle 2| + |\psi_0|^2 |1\rangle\langle 1| + |\psi_-|^2 |0\rangle\langle 0| \qquad (21)$$

the state of L is now in general mixed, so L and R are entangled. We can quantify the entanglement using the purity

$$\mathcal{P} = \mathrm{tr}\, \rho_L^2 = |\psi_+|^4 + |\psi_0|^4 + |\psi_-|^4 \qquad (22)$$

using (20) and writing $q = |\psi_+|^2 = |\psi_-|^2$, we get

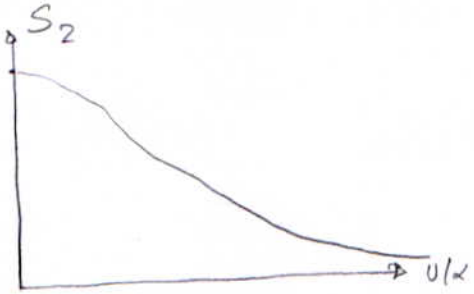
$$\mathcal{P} = q^2 + q^2 + (1 - 2q)^2$$

$$= 1 - 4q + 6q^2$$

$$q = \frac{1}{2} \frac{\alpha^2}{v^2 + \alpha^2} \sin^2 \Omega t.$$

If we plot this, for instance, for $\sin^2 \Omega t = 1/2$, we get something like

It is common to plot the <u>Rényi-2 entropy</u>, $S_2 = -\ln \mathcal{P}$. It would then look like



The tight-binding model

Ok. Warm-up phase is over. Now let's talk about the real deal. This next section is extremely important. We are going to talk about how to deal with quadratic Hamiltonians. That is, Hamiltonians containing only products of two operators.

For instance, in the case of bosons we could have something like

$$H = \sum_{ij} w_{ij} a_i^\dagger a_j \tag{23}$$

where w_{ij} are a set of coefficients. This is not the most general quadratic Hamiltonian. We could also have something like $a_i^\dagger a_j^\dagger + a_i a_j$. But we will not look into those right now.

To have a concrete example in mind, we can talk about a lattice containing only kinetic terms. Assuming for now we are in 1D, we get

The Hamiltonian would then read

$$H = \sum_{i=1}^{L} \epsilon\, a_i^\dagger a_i - J \sum_{i=1}^{L-1} (a_i^\dagger a_{i+1} + a_{i+1}^\dagger a_i) \tag{24}$$

This is called the tight-binding model

By inspection, we can read off what should the matrix W in (23) should be for the Hamiltonian (24); e.g for $L=5$,

$$W = \begin{pmatrix} \epsilon & -J & 0 & 0 & 0 \\ -J & \epsilon & -J & 0 & 0 \\ 0 & -J & \epsilon & -J & 0 \\ 0 & 0 & -J & \epsilon & -J \\ 0 & 0 & 0 & -J & \epsilon \end{pmatrix} \tag{25}$$

this should now start to remind you of our discussion about phonons. The idea is quite similar, except that there we had (q,p) and here we have $(a,a^\dagger)$.

Before we get our hands dirty, let me just mention that this same problem also holds for Fermions. that is, we could consider a quadratic fermionic Hamiltonian of the form

$$H = \sum_{ij\sigma,\sigma'} W_{ij}^{\sigma\sigma'} c_{i\sigma}^\dagger c_{j\sigma'} \tag{26}$$

Now the coefficients W also have a spin index (the 'internal structure'). The tight-binding model (24) would then read

$$H = \sum_{\sigma,i=1}^{L} \epsilon_\sigma c_{i\sigma}^\dagger c_{i\sigma} - J \sum_{\sigma,i=1}^{L-1} (c_{i\sigma}^\dagger c_{i+1,\sigma} + c_{i+1,\sigma}^\dagger c_{i\sigma}) \tag{27}$$

Here I am assuming the hopping J is spin independent, which is a reasonable assumption. You then see that we have essentially two independent tight-binding models, one for each σ.

Going back now to (23), we can diagonalize this Hamiltonian by diagonalizing W. Since $H^\dagger = H$, we must have

$$H^\dagger = \sum_{ij} W_{ij}^* a_j^\dagger a_i = \sum_{ji} W_{ji}^* a_i^\dagger a_j \qquad (28)$$

$$\uparrow$$

$$i \leftrightarrow j$$

Thus we conclude that

$$W_{ji}^* = W_{ij} \quad \text{or} \quad W^\dagger = W \qquad (29)$$

Since W is Hermitian it may be diagonalized by a unitary

$$W_{ij} = \sum_\alpha U_{i\alpha} \varepsilon_\alpha U_{j\alpha}^* \quad \text{or} \quad W = U \varepsilon U^\dagger \qquad (30)$$

Plugging this in (23) we get

$$H = \sum_{ij} \sum_\alpha U_{i\alpha} \varepsilon_\alpha U_{j\alpha}^* a_i^\dagger a_j$$

$$= \sum_\alpha \varepsilon_\alpha \left[\sum_i U_{i\alpha} a_i^\dagger \right] \left[\sum_j U_{j\alpha}^* a_j \right] \qquad (31)$$

This motivates us to define a new set of operators

$$\boxed{\begin{aligned} b_\alpha &= \sum_i U_{i\alpha}^* a_i \\ a_i &= \sum_\alpha U_{i\alpha} b_\alpha \end{aligned}} \qquad (32)$$

(where I used the fact that $U^\dagger U = 1$ to invert the relation in the 2nd line).

with this Eq (31) reduces to

$$\boxed{H = \sum_{\alpha} \varepsilon_\alpha b_\alpha^\dagger b_\alpha} \tag{33}$$

which looks pretty good. But there is a catch. Are the b operators still genuine bosonic operators, like the a's? Recall that

$$[a_i, a_j^\dagger] = \delta_{ij}$$
$$[a_i, a_j] = 0 \tag{34}$$

If this is not the case for the b's, then we will not know how to construct the eigenstates in terms of Fock space.

Well, let's check:

$$[b_\alpha, b_\beta^\dagger] = \sum_{ij} U_{i\alpha}^* U_{j\beta} \underbrace{[a_i, a_j^\dagger]}_{\delta_{ij}} = \sum_i U_{i\alpha}^* U_{i\beta}$$
$$= (U^\dagger U)_{\alpha\beta} = \delta_{\alpha\beta} \tag{35}$$

$$[b_\alpha, b_\beta] = \sum_{ij} U_{i\alpha}^* U_{j\beta}^* \underbrace{[a_i, a_j]}_{0} = 0 \tag{36}$$

Woot! It works. The b's are still bosonic operators.

Incidentally, we have learned a very important lesson:

> Unitary transformations preserve the algebra of the creation and annihilation operators (37)

As a specific example, let us consider the tight-binding model (24). But, as in the case of phonons, let us assume periodic boundary conditions, so that the matrix (25) gets two extra J's on the corners:

$$W = \begin{pmatrix} \epsilon & -J & 0 & 0 & -J \\ -J & \epsilon & J & 0 & 0 \\ 0 & -J & \epsilon & -J & 0 \\ 0 & 0 & -J & \epsilon & -J \\ -J & 0 & 0 & -J & \epsilon \end{pmatrix} \tag{38}$$

Recall from the phonon notes that this is a cyclic matrix and thus may be diagonalized by a Fourier transform (here k takes the role of α in (30))

$$U_{ik} = \frac{1}{\sqrt{L}} e^{ikx_i} \qquad x_i = i \tag{39}$$

$$k = \frac{2\pi \ell}{L} \quad , \quad \ell = 0, \pm 1, \pm 2, \ldots, \pm \frac{L}{2}$$

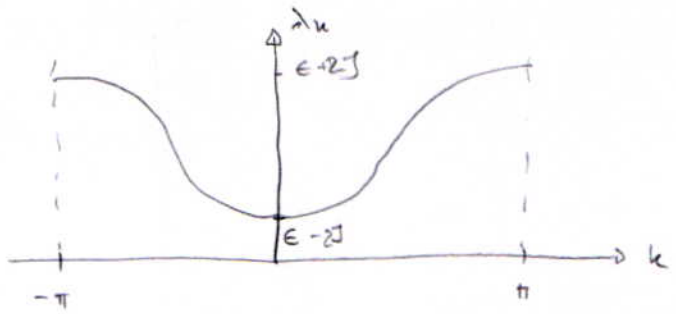
and

$$\boxed{\mathcal{E}_k = \epsilon_0 - 2J \cos k} \tag{40}$$

Thus, the Hamiltonian (24) is diagonalized as

$$H = \sum_k \mathcal{E}_k b_k^\dagger b_k \tag{41}$$

The eigenstates are therefore momentum states, with a dispersion relation given by



this dispersion relation forms what we call an <u>energy band</u>. It says that the eigenstates may lie in a (quasi-) continuum of states going from $\epsilon - 2J$ to $\epsilon + 2J$. The bandwidth is $4J$ (ϵ simply sets the scale of energy).

To construct the eigenstates of H, we can now use the Fock space of the bx. We have the vacuum $|0\rangle$ with no bosons, then the states $|1_k\rangle$ with one boson, then $|1_k, 1_{k'}\rangle$ with 2, and so on.

But now suppose we have exactly N particles in our lattice. What is the ground state? For bosons this answer is insanely easy: just put every one on the state with the smallest possible energy, which is $k = 0$.

$$|gs\rangle = |\text{all } N \text{ particles at } k = 0\rangle$$

This, later on, will be what we will call a <u>Bose-Einstein condensate</u>: a massive condensation of particles into the same quantum state.

We can also do the same for Fermions. The model (27) will have the same matrix W in (38), except that now it will be a W^σ, with ϵ_σ in the diagonals:

$$H = \sum_{ij\sigma} W_{ij}^{\sigma} \, c_{i\sigma}^{\dagger} c_{j\sigma} \tag{42}$$

For each σ we do the same transformation as in (32):

$$d_{k\sigma} = \sum_i U_{ik}^{*} \, c_{i\sigma} = \frac{1}{\sqrt{L}} \sum_i e^{-ikx_i} \, c_{i\sigma} \tag{43}$$

$$c_{i\sigma} = \sum_k U_{ik} \, d_{k\sigma} = \frac{1}{\sqrt{L}} \sum_k e^{ikx_i} \, d_{k\sigma} \tag{44}$$

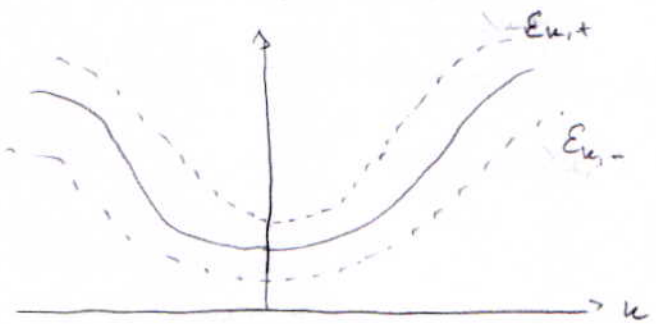
We then get

$$\boxed{H = \sum_{k,\sigma} \varepsilon_{k\sigma} \, d_{k\sigma}^{\dagger} d_{k\sigma}} \tag{45}$$

where

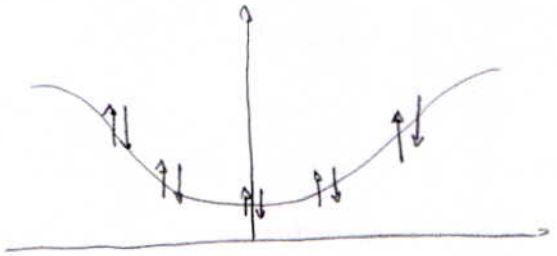
$$\boxed{\varepsilon_{k\sigma} = \epsilon_\sigma - 2J \cos k} \tag{46}$$

Recall that in practice we can have $\epsilon_+ \neq \epsilon_-$ when there is a magnetic field present. Thus we see that for fermions we have 2 bands and the magnetic field may cause a band splitting

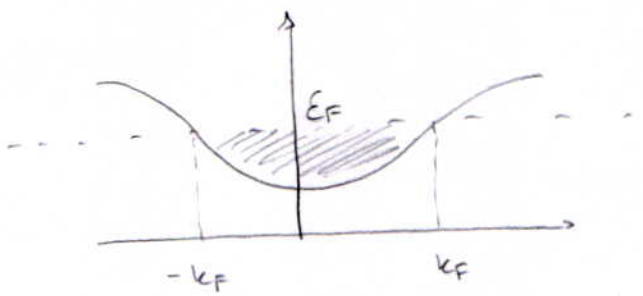


Now let's ask what is the GS when we have N particles. For fermions this question is way more fun because of the exclusion principle. Recall that the matrix W^0 has L eigenstates. That is, L possible values of k. But we have two bands (spin ↑ and spin ↓) so we can accomodate a total of 2L fermions.

So, if we want to talk about ground states, we must fill in the available Fock states from bottom up. First suppose that there is no magnetic field so $\varepsilon_{k\uparrow} = \varepsilon_{k\downarrow}$. Then we will have something like (which is highly exagerated).



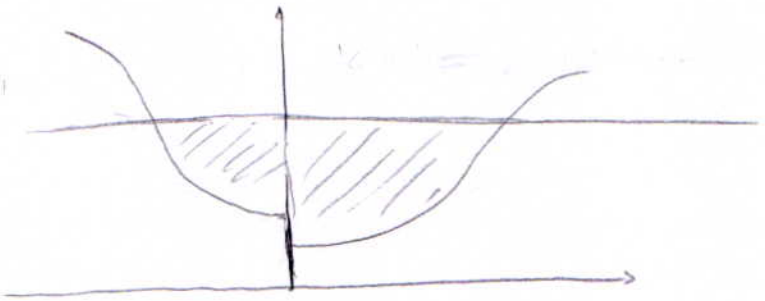
We therefore fill all states with 2 fermions in each, until we fill in N spots. We will therefore start thinking about diagrams such as



we fill the band up to a certain point. For instance, a term which is extensively used in the literature is "Half-filling". This means N = L (one fermion per site).

The energy of the largest filled state is called the Fermi energy ε_F and the corresponding value of k is the Fermi momentum k_F. Any "Fermi" thing always refers to the largest filled state.

Now let's see what happens if we have a magnetic field present. Then we draw a diagram like



(we draw ε_{k+} on the left and ε_{k-} on the right, just for clarity. They actually exist on both $k>0$ and $k<0$). We see from the diagram that in the GS the states with one σ are less filled than the other. Thus, there will be a larger population with one given value of σ. The system will be magnetized.

Multiple orbitals and electronic structure

So far I have been talking a lot about optical lattices and potential wells. But everything we are doing here also applies to electrons in solids or molecules. The idea is really the same. The nuclei create a trap which really looks like the lattices we just studied. There is only one fundamental difference. within each lattice site, the electrons may occupy more than one orbital.

It is easier to think like this: if the atoms were very far apart, the electrons would be able to occupy any of the atomic orbitals available. If we now bring the atoms closer together, this continues to be true, except that now there is also the extra possibility that the electrons tunnel from one site to another.

In the language of 2nd quantization, this means the creation and annihilation operators will have 3 indices

$$c^{+}_{i\sigma\alpha} = \text{creates an } e^- \text{ at site } i, \text{ with spin } \sigma \text{ in the orbital } \alpha \tag{47}$$

Thus, a typical Hamiltonian could look very ugly, like

$$H = \sum_{\substack{ij\sigma\sigma' \\ \alpha\alpha'}} W^{\sigma\sigma'}_{ij\alpha\alpha'} \, c^{+}_{i\sigma\alpha} \, c_{j\sigma'\alpha'} \tag{48}$$

[Yuck!]

Of course, we are not going to do calculations with this guy. I just want us to think for a second about what it means.

So let's draw the following picture

Let's assume there are no magnetic fields. Then W will not depend on σ and only transitions with σ' = σ will be allowed. Eq (48) then simplifies to

$$H = \sum_{\substack{ij\sigma \\ \alpha\alpha'}} W_{ij\alpha\alpha'} \, c^{\dagger}_{i\sigma\alpha} \, c_{j\sigma\alpha'} \tag{49}$$

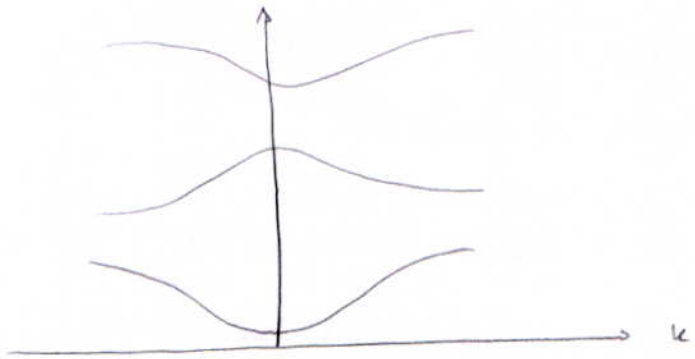
We can also assume the transitions occur mostly between nearest neighbors, as before. Thus, we see that the real new ingredient here is the possibility of tunneling from one orbital α to another α' ≠ α. If the tunneling is small, we could expect that the dominant process is with α' = α. But in real systems α' ≠ α occurs quite often.

If only processes with α' = α survive, then (49) simplifies further to

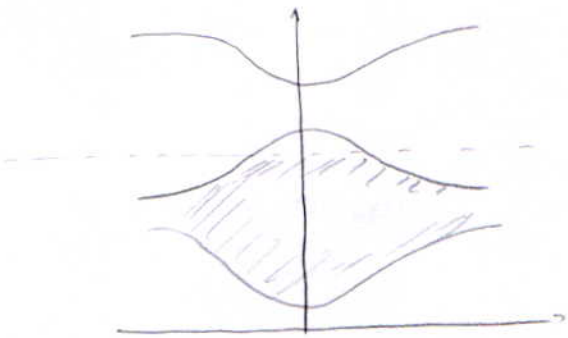
$$H = \sum_{ij\sigma\alpha} W^{\alpha}_{ij} \, c^{\dagger}_{i\sigma\alpha} \, c_{j\sigma\alpha} \tag{50}$$

Now σ and α are just unimportant indices and we can diagonalize H for each α.

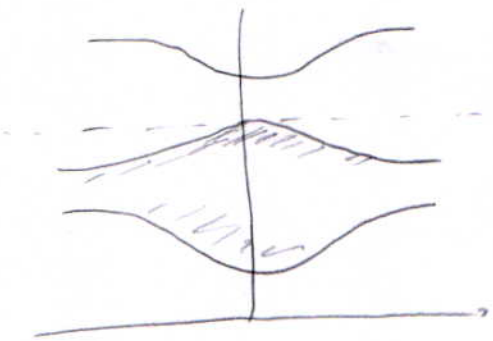
what we will get in the end are then a set of energy bands, one for each α



We now use our rules for filling out the GS, same as before. But notice how now we can have something more interesting, because there are two possible types of ground states



partially filled band



completely filled band

the difference between the two cases lie on the excitations above the ground state. To create an excitation, we remove an electron from a state with $k < k_F$ and put it in a state with $k > k_F$.

But we see that in a partially filled band, there are very many states right above the Fermi level. Hence, the energy cost of creating an excitation.

Conversely, if the band is completely filled, then if we want to create an excitation, it must be on the other band. And there is an energy gap between the bands, so it costs a lot of energy to create the excitation.

What we are talking about here is exactly what differentiates metals and insulators. Metals have partially filled bands so creating excitations is very easy: electrons can move around without difficulty. In an insulator, on the other hand, creating an excitation is hard because there is an energy gap. Consequently it requires a lot of effort to make an electron move.

Electrons and holes

Now I want to show you something quite fun. Suppose we happen to have 2 bands, one filled and one empty:

$$H = \sum_{k,\alpha} \varepsilon_{k\alpha}\, c^{\dagger}_{k\alpha}\, c_{k\alpha} \tag{51}$$

(I'm ignoring spin for simplicity). So we assume that the GS corresponds to the first band being completely filled.

$$|GS\rangle = \left[\prod_{k} c^{\dagger}_{k,1} \right] |0\rangle \tag{52}$$

Now comes a fun idea. Define a new set of operators for band 1 as

$$\boxed{b^{\dagger}_{k,1} := c_{k,1}} \tag{53}$$

this is still a valid fermionic operator, the difference now is that the roles of creation and annihilation are inverted. Thus, instead of saying

$$c_{k,1} = \text{annihilates an electron in band 1} \tag{54}$$

we say

$$b^{\dagger}_{k,1} = \underline{\text{creates}}\ \underline{\text{a}}\ \underline{\text{hole}}\ \text{in band 1} \tag{55}$$

A hole is like the electron's anti-particle. If we remove an electron we leave out a hole. But the hole also behaves like a fermionic particle. In fact, note that

$$c_{k,2}\,|GS\rangle = 0 \tag{56}$$

because band 2 is empty so there is nothing to annihilate.

But

$$c^{\dagger}_{k,1}\,|GS\rangle = 0 \tag{57}$$

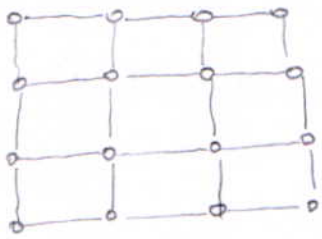
because band 1 is filled already. But in terms of (53), we can write this as

$$b_{k,1}\,|GS\rangle = 0 \tag{58}$$

Thus, we see that the GS behaves like a kind of vacuum for the operators c_{k2} and b_{k1}. Thus, it is like there are two types of particles present: electrons and holes. This is called the Fermi sea: it is a sea from which electron-hole pairs can be created. If you create an electron (ie put an electron in band 2) you must also create a hole (in band 1), which is the electron's anti-particle

Tight-binding on a square lattice

As another example, consider a square lattice with $L \times L$ sites



I will assume we have bosons for now, but the result is the same for Fermions, as we know. For each site we have operators a_{xy}

The tight-binding Hamiltonian then given

$$H = \sum_{x,y} \epsilon\, a^\dagger_{xy} a_{xy} - J \sum_{xy} \left(a^\dagger_{xy} a_{x+1,y} + a^\dagger_{x+1,y} a_{xy} + a^\dagger_{xy} a_{x,y+1} + a^\dagger_{x,y+1} a_{xy} \right) \tag{59}$$

Note how we only include the neighbors which are above or to the right. This way we never double count a bond.

Following what we learned in the 1D case, we now try a transformation of the form

$$b_{\vec{k}} = \frac{1}{\sqrt{L^2}} \sum_{x,y} e^{i(k_x x + k_y y)} a_{xy} \tag{60}$$

where $\vec{k} = (k_x, k_y)$ and each k_i is quantized as in the 1D case

$$k_x = \frac{2\pi \ell_x}{L}, \quad \ell_x = 0, \pm 1, \pm 2, \ldots, \pm \frac{L}{2}$$

$$k_y = \frac{2\pi \ell_y}{L}, \quad \ell_y = 0, \pm 1, \pm 2, \ldots, \pm \frac{L}{2} \tag{61}$$

The inverse transformation is

$$a_{xy} = \frac{1}{L} \sum_{k} e^{i(k_x x + k_y y)} b_k \tag{62}$$

Now it is simply a matter of substituting this in (59) and using the properties of the discrete Fourier transform:

$$\sum_{x,y} a^\dagger_{xy} a_{xy} = \frac{1}{L^2} \sum_{x,y} \sum_{k_x k_y} \sum_{q_x q_y} e^{-i(k_x x + k_y y)} e^{i(q_x x + q_y y)} b^\dagger_k b_q$$

we first carry out the sum over x and y

$$\frac{1}{L^2} \sum_{x,y} e^{i(q_x - k_x)x} e^{i(q_y - k_y)y} = \delta_{q_x, k_x} \delta_{q_y, k_y} \tag{63}$$

Thus

$$\sum_{x,y} a^\dagger_{xy} a_{xy} = \sum_{k_x, k_y} b^\dagger_k b_k \tag{64}$$

(we already saw this kind of result before: it says that the total number of particles is independent of what basis you use)

Next we do the same for the other terms in (59). For instance

$$\sum_{x,y} a^\dagger_{xy} a_{x+1,y} = \frac{1}{L^2} \sum_{x,y} \sum_{k_x k_y} \sum_{q_x q_y} e^{-i(k_x x + k_y y)} e^{i(q_x x + q_y y)} e^{i q_x} \cdot b^\dagger_{k} b_{q}$$

Using (63) again we get

$$\sum_{x,y} a^\dagger_{xy} a_{x+1,y} = \sum_{k_x k_y} e^{i k_x} b^\dagger_{k} b_{k} \tag{65}$$

By taking the adjoint of this result, we also get

$$\sum_{x,y} a^\dagger_{x+1,y} a_{xy} = \sum_{k_x k_y} e^{-i k_x} b^\dagger_{k} b_{k} \tag{66}$$

And, by symmetry, the last 2 terms in (59) should read

$$\sum_{xy} a^\dagger_{xy} a_{x,y+1} = \sum_{k_x k_y} e^{i k_y} b^\dagger_{k} b_{k} \tag{67}$$

$$\sum_{x,y} a^\dagger_{x+1,y} a_{xy} = \sum_{k_x k_y} e^{-i k_y} b^\dagger_{k} b_{k} \tag{68}$$

Thus, combining (64) - (68), we may finally write (59) as

$$H = \sum_{\vec{k}} \left\{ \epsilon - J\left(e^{ik_x} + e^{-ik_x} + e^{ik_y} + e^{-ik_y}\right) \right\} b_{\vec{k}}^{\dagger} b_{\vec{k}} \qquad (69)$$

Thus, if we now define the dispersion relation

$$\boxed{\mathcal{E}_{\vec{k}} = \epsilon - 2J\left(\cos k_x + \cos k_y\right)} \qquad (70)$$

then we finally get

$$\boxed{H = \sum_{\vec{k}} \mathcal{E}_{\vec{k}}\, b_{\vec{k}}^{\dagger} b_{\vec{k}}} \qquad (71)$$

Our energy band now depends on k_x and k_y. You will not be surprised that, if we had instead a 3D lattice, we would get simply

$$\mathcal{E}_{\vec{k}} = \epsilon - 2J\left(\cos k_x + \cos k_y + \cos k_z\right) \qquad (3D) \qquad (72)$$

For small k_x and k_y we may expand the cosines in (70) to get

$$\mathcal{E}_{\vec{k}} \simeq \epsilon - 2J\left(1 - \frac{k_x^2}{2} + 1 - \frac{k_y^2}{2}\right)$$

$$= (\epsilon - 4J) + J(k_x^2 + k_y^2) \tag{73}$$

the term $\epsilon - 4J$ is not really important: it is simply an additive constant. what really matters about this result is that

$$\boxed{\mathcal{E}_{\vec{k}} \simeq J k^2} \qquad k^2 = |\vec{k}|^2 = k_x^2 + k_y^2 \tag{74}$$

this is a typical <u>non-relativistic dispersion relation</u>

$$E = \frac{p^2}{2m} \tag{75}$$

thus, we see that <u>at the bottom of the band</u>, the particles propagate as massive particles, with a mass $m \sim 1/2J$: the higher is the hopping rate J, the lighter is the mass.

Now let's talk about ground-states. For bosons this is again easy. Just put everyone on $(k_x, k_y) = (0,0)$. But for fermions things became more fun. There is a more systematic way of finding the Fermi level which is by means of the implicit equation

$$2 \sum_{\vec{k}} \Theta(\varepsilon_F - \varepsilon_{\vec{k}}) = N \tag{76}$$

where

$$\Theta(x) = \begin{cases} 1 & x > 0 \\ 0 & x < 0 \end{cases} \tag{77}$$

is the Heaviside function. The logic behind (76) is that we should sum over all states and take those for which $\varepsilon_{\vec{k}} < \varepsilon_F$. This ε_F is actually an <u>implicit equation for</u> ε_F. The factor of 2 is to account for the 2 spin configurations.

For large lattices, we can convert the sum in (76) to an integral using the "convenient 1" recipe. Due to (61)

$$\frac{L^2}{(2\pi)^2} \Delta k_x \Delta k_y = 1$$

so

$$2 \sum_{\vec{k}} \Theta(\varepsilon_F - \varepsilon_{\vec{k}}) = \frac{2L^2}{(2\pi)^2} \sum_{\vec{k}} \Delta k_x \Delta k_y \, \Theta(\varepsilon_F - \varepsilon_{\vec{k}})$$

$$= \frac{2L^2}{(2\pi)^2} \int d^2\vec{k} \; \Theta(\varepsilon_F - \varepsilon_{\vec{k}})$$

Thus Eq (76) becomes

$$\frac{2}{(2\pi)^2}\int d^2k\,\Theta(\mathcal{E}_F-\mathcal{E}_k)=\frac{N}{L^2}:=n_0 \tag{78}$$

Note that N/L^2 is the <u>particle density</u> n_0

Let us first suppose that N/L^2 is very small so that we are roughly on the bottom of the band and may approximate $\mathcal{E}_k \simeq Jk^2$.

then we can change variables in (78) to polar coordinates $d^2k = k\,dk\,d\theta$.

Integrating over θ we get

$$n_0 = \frac{2}{(2\pi)^2}\,2\pi\int dk\,k\,\Theta(\mathcal{E}_F - Jk^2)$$

We now define the Fermi momentum from

$$\mathcal{E}_F = J k_F^2 \tag{79}$$

then we get

$$n_0 = \frac{J}{\pi}\int_0^{k_F} dk\,k = \frac{1}{\pi}\,\frac{k_F^2}{2}$$

Hence we get

$$k_F = \sqrt{2\pi n_0} \tag{80}$$

so that the Fermi energy becomes

$$\mathcal{E}_F = J(2\pi n_0) \tag{81}$$

It is also fun to talk about Fermi surfaces. That is, given a certain ε_F, there will be a surface in momentum space corresponding to all values of k such that $\varepsilon_k = \varepsilon_F$.

If $\varepsilon_k = \gamma k^2$, we see that these surfaces will be circles. But for the general dispersion relation (70), these curves will acquire more complicated shapes