

SECOND QUANTIZING THE TIGHT-BINDING HAMILTONIAN

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Reference: Tom Lancaster and Stephen J. Blundell, *Quantum Field Theory for the Gifted Amateur*, (Oxford University Press, 2014), Section 4.3.

As an example of second quantizing the hamiltonian we'll look at a simplified form of the tight-binding model from solid state physics. In a crystal, an electron is typically bound tightly to one particular atom with some energy E which is less than the potential barrier between atoms. However, since the wave functions of two atoms in the lattice will have some overlap, there is always the possibility that an electron can tunnel through the potential barrier and hop from one atom to another. To get a rough idea of what this means, remember that the energy levels of the infinite square well of width a are

$$E_n = \frac{(n\pi\hbar)^2}{2ma^2} \quad (1)$$

As the width of the well increases, the energy levels all decrease so, given a choice, a particle prefers to be in a wider well. Clearly we can't say that the potentials of the electrons in a crystal are infinite square wells since the infinite barriers would prevent hopping altogether, but the same condition is true for the finite square well; a wider well means a lower energy.

The idea behind the tight-binding model is that the ability to tunnel between atoms is favoured by the electron since the wider space available to it results in its energy being lower. The precise amount by which the energy is lowered depends on the nature of the crystal, but for our simple model we'll just say that if an electron tunnels from crystal lattice site j to site l , its energy changes by an amount $-t_{jl}$. This tunneling effect is equivalent (in second quantization language) of annihilating the electron at site j and creating it again at site l , so the portion of the hamiltonian dealing with tunneling can be written as

$$\hat{H} = -\sum_{j,l} t_{jl} c_l^\dagger c_j \quad (2)$$

where c_l^\dagger and c_j are the fermion (since electrons are fermions) creation and annihilation operators.

It's likely that t_{jl} decreases with the separation of the two atoms so as an approximation we can take $t_{jl} = t$ (a constant) for nearest neighbour atoms and $t_{jl} = 0$ for all other atom pairs. Then we get

$$\hat{H} = -t \sum_{l,\tau} c_l^\dagger c_{l+\tau} \quad (3)$$

where the sum over τ means to sum over atoms closest to l .

To diagonalize \hat{H} we can apply Fourier transforms:

$$c_l = \frac{1}{\sqrt{\mathcal{V}}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}_l} c_{\mathbf{k}} \quad (4)$$

$$c_l^\dagger = \frac{1}{\sqrt{\mathcal{V}}} \sum_{\mathbf{q}} e^{-i\mathbf{q}\cdot\mathbf{r}_l} c_{\mathbf{q}}^\dagger \quad (5)$$

Therefore

$$\hat{H} = -\frac{t}{\mathcal{V}} \sum_{l,\tau} \sum_{\mathbf{k},\mathbf{q}} c_{\mathbf{q}}^\dagger c_{\mathbf{k}} e^{i\mathbf{r}_l\cdot(\mathbf{k}-\mathbf{q})} e^{i\mathbf{k}\cdot\mathbf{r}_\tau} \quad (6)$$

We can do the sum over l since

$$\frac{1}{\mathcal{V}} \sum_l e^{i\mathbf{r}_l\cdot(\mathbf{k}-\mathbf{q})} = \delta_{\mathbf{k}\mathbf{q}} \quad (7)$$

[We're summing rather than integrating over \mathbf{r}_l since the atoms are at discrete lattice points in the crystal.] Therefore

$$\hat{H} = -t \sum_{\tau} \sum_{\mathbf{k}} c_{\mathbf{k}}^\dagger c_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}_\tau} \quad (8)$$

$$= \sum_{\mathbf{k}} E_{\mathbf{k}} c_{\mathbf{k}}^\dagger c_{\mathbf{k}} \quad (9)$$

where

$$E_{\mathbf{k}} \equiv -t \sum_{\tau} e^{i\mathbf{k}\cdot\mathbf{r}_\tau} \quad (10)$$

We can see from 9 that \hat{H} is now diagonal in \mathbf{k} -space with eigenvalues $E_{\mathbf{k}}$, so the ground state is the state with the minimum $E_{\mathbf{k}}$.

In a 2-d crystal on a square lattice with the starting atom at the origin, the nearest neighbours are at

$$\mathbf{r}_\tau = (-a, 0), (a, 0), (0, -a), (0, a) \quad (11)$$

so the energy levels are

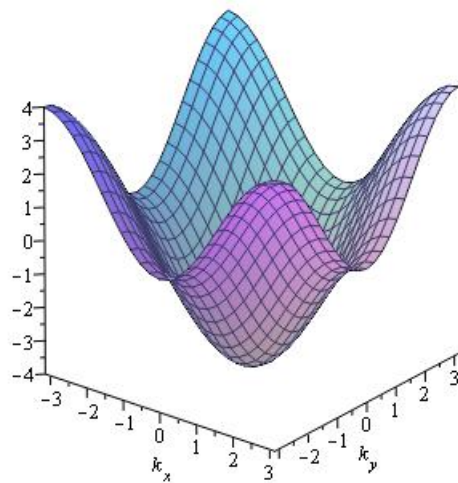
$$E_{\mathbf{k}} = -t \left[e^{ik_x a} + e^{-ik_x a} + e^{ik_y a} + e^{-ik_y a} \right] \quad (12)$$

$$= -2t (\cos(k_x a) + \cos(k_y a)) \quad (13)$$

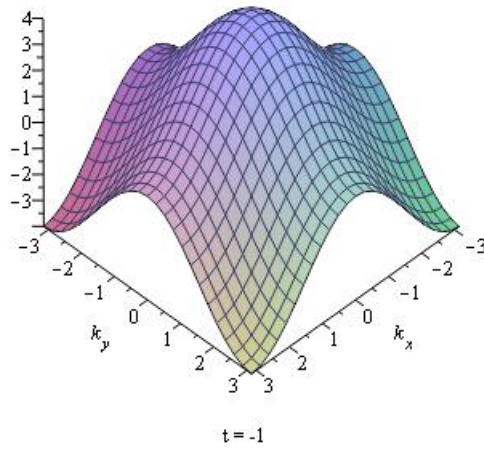
For a 3-d square lattice crystal, we have

$$E_{\mathbf{k}} = -2t (\cos(k_x a) + \cos(k_y a) + \cos(k_z a)) \quad (14)$$

For the 2-d case with $a = 1$ we can plot $E_{\mathbf{k}}$ as a function of k_x and k_y for various values of t . We get:



$t=1$



Keep in mind that the surface is actually a set of discrete points rather than a continuous surface, since \mathbf{k} takes on only discrete values. However, we can see that for $t > 0$ $E_{\mathbf{k}}$ has a minimum at $k_x = k_y = 0$ and for $t < 0$ the minimum occurs at all four corners where $k_x = \pm\pi/a$, $k_y = \pm\pi/a$.