Tight-binding model for electrons in a crystal

Consider a simple crystal, characterized by its atoms being arranged in an ordered way, such that their equilibrium positions are at the sites of a periodic lattice. In the so-called tight-binding model, each electron is taken to be in an orbital localized around a particular atom[1] and has a (small) amplitude for tunneling to a different orbital localized around a nearby atom. For simplicity let us assume that only one orbital per atom is relevant for this conduction and furthermore that the crystal is one-dimensional (1D).[2] Consider therefore a 1D lattice with N sites.[3] Let the operator $\hat{c}^\dagger_{j\sigma}$ create an electron in the orbital localized around site $j = 1, 2, \ldots, N$ with spin projection $\sigma = \pm 1/2$. We will use periodic boundary conditions, i.e. $\hat{c}_{j+N,\sigma} = \hat{c}_{j,\sigma}$, which makes the system like a necklace, with the sites being "beads" evenly spaced along it. Let us consider the following Hamiltonian:

$$\hat{H} = -t \sum_{j,\sigma} (\hat{c}^\dagger_{j,\sigma} \hat{c}_{j+1,\sigma} + \text{h.c.}) \tag{1}$$

where "h.c." means hermitian conjugate, i.e. the adjoint operator. This Hamiltonian is the kinetic energy operator associated with the electrons hopping between neighbouring sites on the 1D lattice. To see this, consider an electron with spin σ sitting on site ℓ and consider the process of this electron hopping to the site immediately to the right, which has label $\ell + 1$. So in the initial state this electron is on site ℓ while in the final state it has moved to site $\ell + 1$. Mathematically, the hopping can be described as a two-step process: First the electron with spin σ at site ℓ is annihilated, and then the electron with spin σ at site $\ell + 1$ is created. This is effected by the operator $\hat{c}^\dagger_{\ell+1,\sigma} \hat{c}_{\ell,\sigma}$. Its h.c. describes the hopping of an electron with spin σ from site $\ell + 1$ to site ℓ. The parameter $t > 0$ is called the hopping amplitude.[4]

We want to find the eigenstates and eigenvalues of $\hat{H}$. To this end, we introduce operators creating and annihilating electrons in definite k-states[5] by writing

$$\hat{c}_{j\sigma} = \frac{1}{\sqrt{N}} \sum_k e^{ikr_j} \hat{c}_{k\sigma}, \tag{2}$$

[1] Technically, these orbitals are called Wannier orbitals. They form a complete orthonormal basis.

[2] For a general and careful discussion of the tight-binding model, see Ch. 10 of Ashcroft and Mermin, "Solid state physics", Thomson Learning, 1976.

[3] Please note that in this section N stands for the number of sites, while in the previous section N was the number of electrons, which in this section will be called N_e....

[4] For a more detailed discussion, see Sec. 3.1 in Nagaosa's "Quantum field theory in strongly correlated electronic systems" and Sec. 2.2 in "Condensed matter field theory" by Altland and Simons (p. 54-55). In our discussion we will just take t as a given parameter.

[5] More precisely, the state created (annihilated) by $\hat{c}^\dagger_{k\sigma}$ ($\hat{c}_{k\sigma}$) is called a Bloch state. Its wavevector k is restricted to the 1st Brillouin zone (see below). It can be shown that the wave function of a Bloch state can be written as the product of a plane wave (with wave vector k) and a function with the periodicity of the crystal lattice (this fact is however not needed in the following discussion).

where

$$r_j = ja \tag{3}$$

is the position of site j in the lattice, where a is the distance between neighbouring sites (a is usually called the lattice constant). The total length of the system is $L = Na$. Periodic boundary conditions $\hat{c}_{j\sigma} = \hat{c}_{j+N,\sigma}$ imply that $e^{ikL} = 1$, i.e. the allowed wavevectors take the form $k = 2\pi m/L$ where m is an integer. Because we have (for each value of σ) N operators $\hat{c}_{j\sigma}$ (since $j = 1, 2, \ldots, N$), we also have N independent operators $\hat{c}_{k\sigma}$ corresponding to N inequivalent values of k. It is customary to choose these N k-values to be given by $m = -N/2, -N/2+1, \ldots, N/2-1$ (here we assumed that N is an even number). This gives $k = -\pi/a, -\pi/a + 2\pi/L, \ldots, \pi/a - 2\pi/L$, which in the limit $N \to \infty$ means that k lies in the region $[-\pi/a, \pi/a\rangle$ which is called the 1st Brillouin zone for the 1D lattice. The inverse transformation is

$$\hat{c}_{k\sigma} = \frac{1}{\sqrt{N}} \sum_j e^{-ikr_j} \hat{c}_{j\sigma}. \tag{4}$$

This can be seen by checking that the transformation and the inverse transformation "undo" each other, thus taking us back to where we started:

$$\begin{aligned} \hat{c}_{j\sigma} &= \frac{1}{\sqrt{N}} \sum_k e^{ikja} \hat{c}_{k\sigma} = \frac{1}{\sqrt{N}} \sum_k e^{ikja} \frac{1}{\sqrt{N}} \sum_{j'} e^{-ikj'a} \hat{c}_{j'\sigma} \\ &= \sum_{j'} \hat{c}_{j'\sigma} \underbrace{\frac{1}{N} \sum_k e^{ik(j-j')a}}_{\delta_{jj'} \text{(see Appendix)}} = \sum_{j'} \hat{c}_{j'\sigma} \delta_{jj'} = \hat{c}_{j\sigma}. \end{aligned} \tag{5}$$

Note that $\hat{c}_{k+2\pi/a,\sigma} = \hat{c}_{k\sigma}$, which shows that wavevectors that differ by an integer multiple of $2\pi/a$ are equivalent to each other. This is of course consistent with our finding above that we could choose the N inequivalent values of k to all lie inside the 1st Brillouin zone, an interval of length $2\pi/a$. Using the anticommutation relations for the site-labeled operators, i.e.

$$\{c_{j\sigma}, c^\dagger_{j'\sigma'}\} = \delta_{jj'}\delta_{\sigma\sigma'}, \quad \{c_{j\sigma}, c_{j'\sigma'}\} = \{c^\dagger_{j\sigma}, c^\dagger_{j'\sigma'}\} = 0, \tag{6}$$

one finds that the wavevector-labeled operators satisfy the same kind of canonical anticommutation relations, i.e.

$$\{c_{k\sigma}, c^\dagger_{k'\sigma'}\} = \delta_{kk'}\delta_{\sigma\sigma'}, \quad \{c_{k\sigma}, c_{k'\sigma'}\} = \{c^\dagger_{k\sigma}, c^\dagger_{k'\sigma'}\} = 0. \tag{7}$$

Using the transformation (2) the sum $\sum_j \hat{c}^\dagger_{j\sigma}\hat{c}_{j+1,\sigma}$ appearing in $\hat{H}$ becomes

$$\begin{aligned} \sum_j \hat{c}^\dagger_{j\sigma}\hat{c}_{j+1,\sigma} &= \frac{1}{N} \sum_j \sum_{k,k'} e^{-ikja} e^{ik'(j+1)a} \hat{c}^\dagger_{k\sigma}\hat{c}_{k'\sigma} \\ &= \sum_{k,k'} \hat{c}^\dagger_{k,\sigma}\hat{c}_{k'\sigma} e^{ik'a} \underbrace{\frac{1}{N} \sum_j e^{-i(k-k')ja}}_{\delta_{kk'} \text{(see Appendix)}} \\ &= \sum_k e^{ika}\ \hat{c}^\dagger_{k\sigma}\hat{c}_{k\sigma}. \end{aligned} \tag{8}$$

Thus

$$\hat{H} = -t\sum_{k,\sigma}(e^{ika}\ \hat{c}^{\dagger}_{k\sigma}\hat{c}_{k\sigma} + \text{h.c.}) = -t\sum_{k,\sigma}(e^{ika} + e^{-ika})\hat{c}^{\dagger}_{k\sigma}\hat{c}_{k\sigma}, \tag{9}$$

i.e.

$$\hat{H} = \sum_{k\sigma}\varepsilon_k \hat{c}^{\dagger}_{k\sigma}\hat{c}_{k\sigma}, \tag{10}$$

where the energy function ε_k, often called the *dispersion relation*, is given by

$$\varepsilon_k = -2t\cos ka. \tag{11}$$

Eq. (10) gives $\hat{H}$ as a linear combination of number operators $\hat{n}_{k\sigma} = \hat{c}^{\dagger}_{k\sigma}\hat{c}_{k\sigma}$. The eigenstates and eigenvalues of $\hat{H}$ can then be read off easily. An arbitrary eigenstate $|A\rangle$ of $\hat{H}$ is specified by giving its occupation numbers $n^{(A)}_{k,\sigma}$ ($= 0$ or 1) for all the single-particle state (k, σ). The associated eigenvalue E_a is given by

$$E_a = \sum_{k\sigma\in A}\varepsilon_k \tag{12}$$

where the sum runs over those (k, σ) states that are occupied in $|A\rangle$ (i.e. have $n^{(A)}_{k\sigma} = 1$).

Typically we are interested in a system which contains some fixed number of electrons N_e (note that we must have $N_e \leq 2N$ due to the Pauli principle). The occupation numbers $n_{k,\sigma}$ of an eigenstate with N_e electrons therefore satisfies the constraint

$$\sum_{k,\sigma} n_{k,\sigma} = N_e. \tag{13}$$

The ground state of such a system is obtained by filling those N_e (k, σ) states that have the smallest energy ε_k. Each k-state can be occupied by two electrons, one having $\sigma = +1/2$ (spin $\uparrow$) and the other having $\sigma = -1/2$ (spin $\downarrow$). As ε_k has a minimum at $k = 0$ and grows monotonically as k moves away from 0 inside the 1st Brillouin zone, the k-states that will be filled are the $N_e/2$ states closest to $k = 0$, which will enclose a region from $k = -k_F$ to $k = +k_F$ where k_F is the Fermi wavevector. Thus the ground state can again be written on the form $\prod_{|k|<k_F}\hat{c}^{\dagger}_{k\uparrow}\hat{c}^{\dagger}_{k\downarrow}|0\rangle$, and the relationship between the particle density n and k_F can be worked out in a similar way as for the free electron gas (and so can the relationship between the ground state energy E_0 and k_F).

So far we have considered electrons hopping on a 1D lattice. Of course, electrons hopping on 2- or 3-dimensional lattices is at least as relevant, and it is straightforward to generalize the hopping Hamiltonian (1) to such higher-dimensional lattices. In this course we limit ourselves to "hypercubic" lattices, i.e. a square lattice in two dimensions and a cubic lattice in three dimensions. Then the associated 1st Brillouin zone becomes a square in two dimensions and a cube in three dimensions, centered at the origin in k-space and with sides of length $2\pi/a$ parallel to the axes of the real-space lattice. Note that when discussing lattice problems like these, one very often chooses to measure distances in units of the lattice spacing a, thus setting $a = 1$. Then wavevectors become dimensionless, so the sides of the 1st Brillouin zone have length 2π (i.e. running from $-\pi$ to π in each of the D k-space directions for a D-dimensional lattice).

A Some frequently encountered k- and j-sums

In these notes we used that

$$\sum_k e^{ik(j-j')a} = N\delta_{jj'}, \tag{14}$$

$$\sum_j e^{-i(k-k')ja} = N\delta_{kk'}, \tag{15}$$

where $k = 2\pi m/L$ and $k' = 2\pi m'/L$, with m and m' integers that can take the values $-N/2, \ldots, N/2-1$ such that k and k' are in the 1st Brillouin zone $[-\pi/a, \pi/a\rangle$, and $j = 1, 2, \ldots N$.

Let us prove Eq. (14). If $j = j'$ the exponential is 1, so the sum is $N \cdot 1 = N$. If $j \neq j'$, consider the summand which is

$$e^{ik(j-j')a} = e^{i\frac{2\pi}{Na}m(j-j')a} \equiv x^m, \qquad \text{where } x \equiv e^{i2\pi(j-j')/N}. \tag{16}$$

Since both j and j' can only take values between 1 and N, and we have assumed $j \neq j'$, we get $0 < |j - j'| < N$, and therefore $x \neq 1$. We now rewrite the sum as

$$\sum_k e^{ik(j-j')a} = \sum_{m=-N/2}^{N/2-1} x^m = x^{-N/2} \sum_{m=0}^{N-1} x^m = x^{-N/2} \frac{1-x^N}{1-x}, \tag{17}$$

where we used the formula for the sum of a geometric series. Since $x \neq 1$ the denominator $1-x$ is nonzero. Furthermore, $x^N = e^{i2\pi(j-j')} = 1$, so $1-x^N$ vanishes. This proves Eq. (14).

The proof of (15) is very similar and is therefore left to the reader.