QFT by Lancaster and Blundell Section 4.3

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Physics Cafe

June 27, 2021

Outline

4.3 The Kinetic Energy and Tight-Binding Hamiltonian

- To start with, recall the Hamiltonian of a free particle we derived earlier in terms of creation and annihilation operators of momentum states,

$$\hat{H}_{\text{free}} = \sum_p \frac{p^2}{2m} \hat{a}_p^\dagger \hat{a}_p \tag{1}$$

$$= \sum_k \frac{\hbar^2 k^2}{2m} \hat{a}_k^\dagger \hat{a}_k \tag{2}$$

$$\equiv \sum_k E_k^{\text{free}} \hat{a}_k^\dagger \hat{a}_k. \tag{3}$$

- We can express this in position space using the position-momentum Fourier relations

$$\hat{a}_k^\dagger = \sum_j e^{ik\cdot x_j} \hat{a}_j^\dagger \tag{4}$$

$$\hat{a}_k = \sum_j e^{-ik\cdot x_j} \hat{a}_j \tag{5}$$

that we showed in equations (48) and (49) of the previous slides.

- Substituting in we have,

$$\hat{H}_{\text{free}} = \sum_{ij} \sum_{k} E_k^{\text{free}} e^{ik\cdot(r_i - r_j)} \hat{a}_k^\dagger \hat{a}_k. \tag{6}$$

Defining

$$t_{ij} = \sum_{k} E_k^{\text{free}} e^{ik\cdot(r_i - r_j)} \tag{7}$$

we can write the Hamiltonian as,

$$\hat{H}_{\text{free}} = \sum_{ij} t_{ij} \hat{a}_k^\dagger \hat{a}_k. \tag{8}$$

- Now consider the case where these non-interacting fermions live on a crystal lattice with a potential well located at each of the lattice sites.

- The particles will now tend to become more localized to the lattice sites and it will be harder for one to "hop" to sites that are far away (t_{ij} will be very small if $\|r_i - r_j\|$ is large).

- In the tight-binding approximation, we assume

$$t_{ij} = \begin{cases} -t, & i,j \text{ are nearest neighbours.} \\ 0, & \text{otherwise.} \end{cases} \tag{9}$$

- For example, with four points $(1, 2, 3, 4)$ arranged consecutively with periodic boundary conditions so that points 1 and 4 connect with each other.

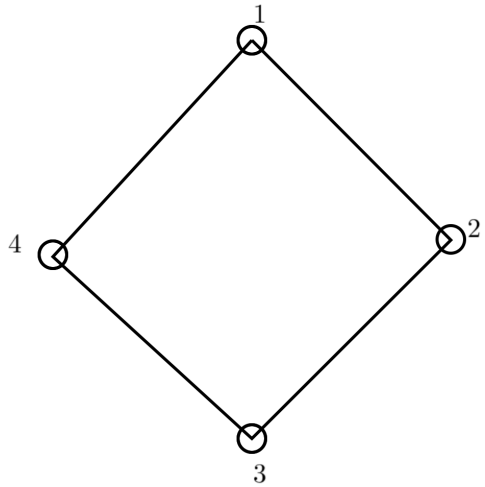

Figure: Four crystal sites arranged with PBC's.

- The nearest neighbour pairs in the original sum would be,

$$\begin{array}{lcccc} \text{Site No.} & \textcircled{1} & \textcircled{2} & \textcircled{3} & \textcircled{4} \\ & (12) & (21) & (32) & (43) \\ & (14) & (23) & (34) & (41) \end{array} \tag{10}$$

- This gives us the tight-binding Hamiltonian,

$$H_{tb} = -t \sum_{\langle ij \rangle} \hat{a}_i^\dagger \hat{a}_j + \hat{a}_j^\dagger \hat{a}_j, \tag{11}$$

where the $\langle ij \rangle$ denote all nearest neighbour pairs.

- The set of nearest neighbour pairs in the new notation are $< 12 >, < 23 >, < 34 >, < 41 >$.

- We can now rewrite the sum as a sum over sites first and then a sum over the site's nearest neighbours,

$$H_{tb} = -t \sum_{\langle ij \rangle} \hat{a}_i^\dagger \hat{a}_j + \hat{a}_j^\dagger \hat{a}_j \tag{12}$$

$$\boxed{H_{tb} = \frac{1}{2} \sum_i \sum_\tau \hat{a}_i^\dagger \hat{a}_{i+\tau} + \hat{a}_{i+\tau}^\dagger \hat{a}_i}, \tag{13}$$

  where the sum over τ is carried over the nearest neighbour offset vectors $\tau_1, \tau_2, \ldots, \tau_q$.

- Here q is the number of nearest neighbours in the particular lattice we are considering (e.g., two for a one dimensional uniform lattice, four for a two dimensional square lattice, six for a three dimensional cubic, etc.).

- The operator $\hat{a}_{i+\tau}$ annihilates a particle in at the site $r_{i+\tau}$ while $\hat{a}_i^\dagger$ creates a particle at site r_i.
  The factor of $\frac{1}{2}$ avoids double counting.

- What is important here when we rewrite the Hamiltonian in terms of a sum over sites plus a sum over neighbours for each site is that *cyclic symmetry* of the Hamiltonian is revealed.

- You can see this explicitly in the one dimensional single particle case of a uniform lattice containing one particle with periodic boundary conditions.

- The state of the system with a particle at site i is denoted $|i\rangle$.

- You can see from inspection the destruction/creation combination of $\hat{a}_i^\dagger \hat{a}_{i+1} = |i\rangle\langle i+1|$, $\hat{a}_i^\dagger \hat{a}_{i-1} = |i\rangle\langle i-1|$, and similar for $\hat{a}_{i+\tau}^\dagger \hat{a}_i$ for the two values of $\tau = \pm 1$.

- So we can write the Hamiltonian as,

$$H_{tb} = -t \sum_{i=1}^{N} |i\rangle\langle i+1| + |i+1\rangle\langle i|. \tag{14}$$

- We removed the $i-1$ bra's and ket's by double counting and removing the factor of $\frac{1}{2}$.

- Assuming PBC means the sum goes up to $i = N$.
  This means that a term $|N\rangle\langle N+1|$ should be interpreted as $|N\rangle\langle 1|$.

- When a term like $|i+1\rangle\langle i|$ acts on a state $|i\rangle$ it produces $|i+1\rangle$.
  Thus, $|i+1\rangle\langle i|$ describes a jump from i to $i+1$ (you read it from right to left).

- So what does the operator H_{tb} look like as a matrix in the particle position basis $|i\rangle$ for a particular lattice size N? Take $N = 5$. Then,

$$H_{tb} = -t \begin{pmatrix} 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 \end{pmatrix} \tag{15}$$

- The particular symmetry of the matrix where every row is a shifted version of the previous one is know as *circulant*.

- A remarkable property of circulant matrices is they can be diagonalized by a Fourier transform matrix. The eigenvectors are always the same regardless of the actual entries of the matrix, as long as it has this row shifted symmetry.

- This is used often in signal processing where linear filters can be represented by circulant matrices. This is why the discrete Fourier transform has such widespread use.

- So let's Fourier transform our Hamiltonian by taking it's representation in the momentum basis. We start with

$$H_{tb} = \frac{1}{2}\sum_i \sum_\tau \hat{a}_i^\dagger \hat{a}_{i+\tau} + \hat{a}_{i+\tau}^\dagger \hat{a}_i \tag{16}$$

- Now perform the substitutions,

$$\hat{a}_j^\dagger \leftarrow \frac{1}{\sqrt{N}}\sum_k e^{-ik\cdot x_j}\hat{a}_k^\dagger \tag{17}$$

$$\hat{a}_j \leftarrow \frac{1}{\sqrt{N}}\sum_k e^{ik\cdot x_j}\hat{a}_k \tag{18}$$

- This gives us,

$$H_{tb} = -\frac{t}{2N}\sum_i \sum_{\tau,k,k'} e^{-ik\cdot r_i} e^{ik'\cdot(r_i+\tau)}\hat{a}_k^\dagger \hat{a}_{k'} + e^{-ik'\cdot(r_i+\tau)} e^{ik\cdot r_i}\hat{a}_k^\dagger \hat{a}_{k'} \tag{19}$$

$$= -\frac{t}{2N}\sum_i \sum_{\tau,k,k'} e^{ir_i\cdot(k'-k)} e^{ik'\tau}\hat{a}_k^\dagger \hat{a}_{k'} + e^{-ir_i\cdot(k'-k)} e^{-ik'\tau}\hat{a}_k^\dagger \hat{a}_{k'} \tag{20}$$

$$= -\frac{t}{2N}\sum_{k,\tau}(e^{ik'\tau} + e^{-ik'\tau})\hat{a}_k^\dagger \hat{a}_{k'} \cdot \underbrace{\sum_{i,k'} e^{ir_i(k-k')}}_{N\cdot\delta_{kk'}} \tag{21}$$

$$= -t\sum \cos(k\cdot\tau)\hat{a}_k^\dagger \hat{a}_k \tag{22}$$

- So we can write the Hamiltonian in the diagonal form,

$$H_{tb} = \sum_k E_k^{tb} \hat{a}_k^\dagger \hat{a}_k \tag{23}$$

where the energies are given by

$$E_k^{tb} = -t \sum_\tau \cos(k \cdot \tau). \tag{24}$$

- This is the system's *dispersion* relation between energy and momentum. Compare this to the free particle

$$E_k^{free} = \frac{\hbar^2}{2m} k^2. \tag{25}$$

- We see that in a lattice the energy is now bounded with respect to its wavenumber, unlike a free particle.

Example (1-D Chain)

- For a one-dimensional chain the nearest neighbour vectors are $\tau_1 = a$ and $\tau = -a$ where a is the lattice spacing.

- The energy dispersion relation is then,

$$E_k^{tb} = -t\left[\cos(ka) + \cos(-ka)\right] \tag{26}$$

$$= -2t\cos(ka). \tag{27}$$

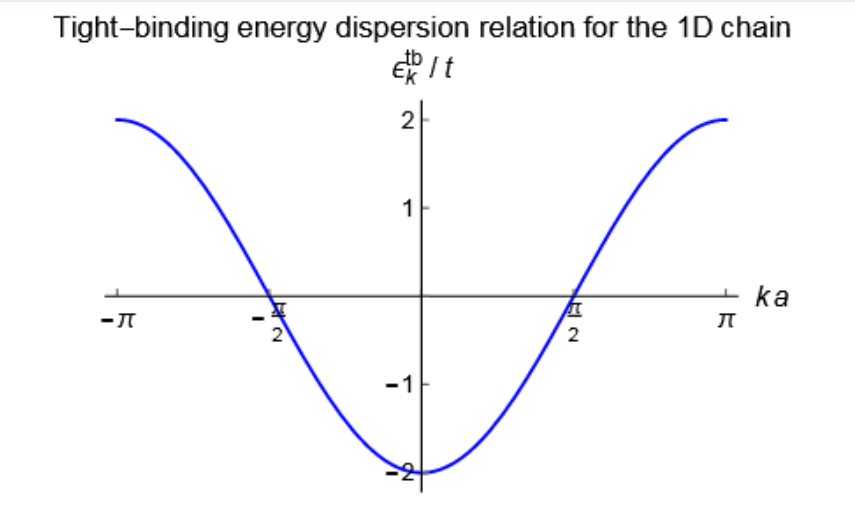

Figure: Dispersion relation for 1-D tight binding model.

- The tight-binding Hamiltonian is then,

$$H_{tb} = -2t\sum_k \cos(ka)\cdot \hat{a}_k^\dagger \hat{a}_k \tag{28}$$

Example (2-D Square Lattice)

- Now we have four nearest neighbour displacement vectors with lattice spacing a,

$$\tau_1 = a\hat{x},\ \tau_2 = -a\hat{x},\ \tau_3 = a\hat{y},\ \tau_4 = a\hat{y}. \tag{29}$$

- The energy dispersion relation is now,

$$E_k^{tb} = -t\left[\cos(k_x a) + \cos(-k_x a) + \cos(k_y a) + \cos(-k_y a)\right] \tag{30}$$

$$= -2t\left[\cos(k_x a) + \cos(k_y a)\right]. \tag{31}$$

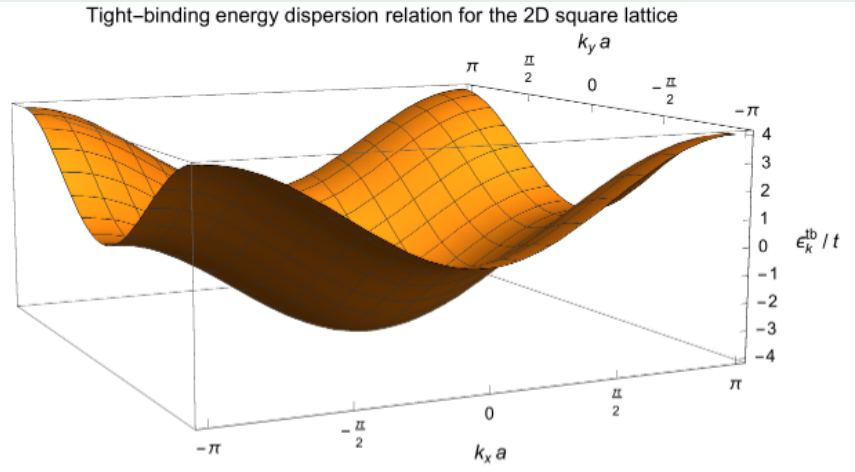

Figure: Dispersion relation for 1-D tight binding model.

- The tight-binding Hamiltonian is then,

$$H_{tb} = -2t \sum_k \left[\cos(k_x a)\cos(k_y a)\right] \cdot \hat{a}_k^\dagger \hat{a}_k \tag{32}$$