Summer Project on Condensed Matter Physics - IISc, Bangalore 2023

Lecture 2: Solution of Tight-Binding Model Hamiltonian

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In this lecture, the tight-binding hamiltonian for a periodic 1-D lattice was solved.

1 Tight-Binding Model for Periodic 1-D Lattice

Consider the Hamiltonian:

$$H = \sum_{n=1}^{\infty} E_0 c_n^\dagger c_n - \sum_{n=1}^{\infty} \gamma (c_n^\dagger c_{n+1} + c_{n+1}^\dagger c_{n+1}) \tag{1}$$

The most pertinent question we need to answer is: what are the eigenstates and eigenvalues of this Hamiltonian? It is better understood as follows: The number states $|n\rangle$ for a given pair of creation and annihilation operators will be used to construct the eigenstates as the Hamiltonian is itself a sum of various $c_n^\dagger$'s and c_n's.
Also, we will use periodic boundary conditions i.e., $c_{N+1} = c_1$. Now let us see what happens when the Hamiltonian H acts on a state $|n\rangle$.
From the anticommutator relation of c_m and $c_n^\dagger$, we get;

$$c_m c_n^\dagger = -c_n^\dagger c_m + \delta_{mn} \tag{2}$$

Thus we get:

$$c_m |n\rangle = c_m c_n^\dagger |vac\rangle \tag{3}$$
$$= (-c_n^\dagger c_m + \delta_{mn}) |vac\rangle \tag{4}$$
$$= \delta_{mn} |vac\rangle \tag{5}$$

The different parts of the Hamiltonian act as follows:

$$-\gamma \sum_m (c_m^\dagger c_{m+1} + c_{m+1}^\dagger c_m) |n\rangle = - - \gamma \sum_m (c_m^\dagger \delta m+1, m + c_{m+1}^\dagger \delta m, n) |vac\rangle \tag{6}$$
$$= -\gamma (c_{n-1}^\dagger + c_{n+1}^\dagger) |vac\rangle \tag{7}$$
$$= \gamma (|n+1\rangle + |n-1\rangle \tag{8}$$

$$E_0 \sum_m c_m^\dagger c_m |n\rangle = E_0 \sum_m c_m^\dagger \delta_{m,n} |vac\rangle \tag{9}$$
$$= E_0 |n\rangle \tag{10}$$

Therefore,

$$H |n\rangle = -\gamma (|n+1\rangle |n-1\rangle) + E_0 |n\rangle \tag{11}$$

2 Eigenstates and Eigenvalues

Next, we are going to use translational invariance of the system to look for plane wave eigenstates of the Hamiltonian. This just means that if the Hamiltonian is invariant under $n \to n+1$ then the eigenstates can be expected to be of the form of plane waves. Thus, try:

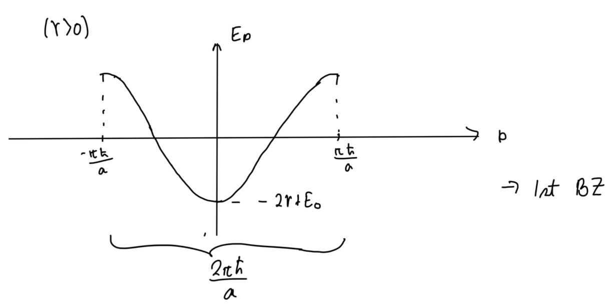
$$|p\rangle = \sum_{n=1}^{N} e^{\frac{ipna}{\hbar}} |n\rangle \tag{12}$$

Then,

$$\begin{aligned}
H|p\rangle &= \sum_{n=1}^{N} e^{\frac{ipna}{\hbar}} H|n\rangle && (13)\\
&= \sum_{n=1}^{N} e^{\frac{ipna}{\hbar}} \left(\gamma |n+1\rangle\, \gamma |n-1\rangle + E_0 |n\rangle\right) && (14)\\
&= \sum_{n} \left(e^{\frac{ip(n-1)a}{\hbar}}(-\gamma)|n\rangle + e^{\frac{ip(n+1)a}{\hbar}}(-\gamma)|n\rangle + e^{\frac{ipna}{\hbar}} E_0 |n\rangle\right) && (15)\\
&= \sum_{n} e^{\frac{ipna}{\hbar}} |n\rangle \left[-\gamma e^{\frac{-ipa}{\hbar}} - \gamma e^{\frac{ipa}{\hbar}} + E_0\right] && (16)\\
&= \sum_{n} e^{\frac{ipna}{\hbar}} |n\rangle \left[E_0 - 2\gamma cos\left(\frac{pa}{\hbar}\right)\right] && (17)\\
&= |p\rangle \left[E_0 - 2\gamma cos\left(\frac{pa}{\hbar}\right)\right] && (18)
\end{aligned}$$

$$\begin{aligned}
\therefore H|p\rangle &= \left[E_0 - 2\gamma cos\left(\frac{pa}{\hbar}\right)\right]|p\rangle && (19)\\
&= E_p |p\rangle && (20)
\end{aligned}$$

$\implies |p\rangle$ is an eigenstate of H with an eigenvalue : $E_p = E_0 - 2\gamma cos\left(\frac{pa}{\hbar}\right)$.



But now, we must think of how many values of p are allowed?

$$|p\rangle = \sum_n e^{\frac{ipna}{\hbar}|n\rangle}$$

The coefficients of $n = N + 1$ and $n = 1$ are the same.

$$\implies e^{\frac{ipa(N+1}{\hbar}} = e^{\frac{ipa}{\hbar}} \implies e^{\frac{ipNa}{\hbar}}] = 1$$

Therefore, p is quantized in units of $\frac{2\pi\hbar}{aN}$.
$p = \frac{2\pi\hbar}{aN}$ times some integer.
(Always the case that no. of modes in real space = no. of modes in Fourier space!)

3 (Anti!)commutators in Fourier Space

In the last section we did something funny with how we defined the eigenstate of the Hamiltonian given by Eq (1). We took a sum of plane wave solutions over all the allowed values of n. Something like this is done very frequently when we deal with Fourier series. So we should be able to get the solution we obtained above by taking a Fourier series of something. That something will be the creation and annihilation operators we defined in Lecture 1. What we will do is convert the creation and annihilation operators from the number space to Fourier space i.e., k-space[1] via a discrete Fourier transform.
The Fourier transforms will be deifned as follows:

$$c_p = \frac{1}{\sqrt{N}} \sum_n e^{\frac{-ipna}{\hbar}} c_n \tag{21}$$

$$c_n = \frac{1}{\sqrt{N}} \sum_n e^{\frac{ipna}{\hbar}} c_p \tag{22}$$

$$c_p^\dagger = \frac{1}{\sqrt{N}} \sum_n e^{\frac{ipna}{\hbar}} c_n^\dagger \tag{23}$$

$$c_n^\dagger = \frac{1}{\sqrt{N}} \sum_n e^{\frac{-ipna}{\hbar}} c_p^\dagger \tag{24}$$

We know the anticommutator relations in number space from Lecture 1:

$$\{c_m^\dagger, c_n^\dagger\} = 0 \tag{25}$$

$$\{c_m, c_n\} = 0 \tag{26}$$

$$\{c_m, c_n^\dagger\} = \delta_{mn} \tag{27}$$

[1]Here it is p-space but k and p are related.

We can show that in p-space, the anticommutator relations are:

$$\{c_p^\dagger, c_{p'}^\dagger\} = 0 \tag{28}$$
$$\{c_p, c_{p'}\} = 0 \tag{29}$$
$$\{c_p, c_{p'}^\dagger\} = \delta_{pp'} \tag{30}$$

Let's see what these new operators do. Consider a vacuum state $|vac\rangle$. Act the new operators on this state. We get:

$$c_p |vac\rangle = 0 \tag{31}$$
$$c_p^\dagger |vac\rangle = |p\rangle \tag{32}$$
$$c_{p_1}^\dagger c_{p_2}^\dagger |vac\rangle = |p_1, p_2\rangle \tag{33}$$
$$c_{p_2}^\dagger c_{p_1}^\dagger |vac\rangle = |p_2, p_1\rangle = -|p_1, p_2\rangle \tag{34}$$