Summer Project on Condensed Matter Physics - IISc, Bangalore 2023

Lecture 6: Dirac Equation in Condensed Matter Systems

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The necessity of the Dirac equation in condensed matter systems was elucidated in this lecture.

1 Relativistic Dispersion in Non-relativistic Systems

We know that the Dirac equation is the fundamental equation in relativistic quantum mechanics just like Schrodinger's equation is the fundamental equation in non-relativistic quantum mechanics. The Dirac equation demands a relativistic dispersion relation:

$$E^2 = \vec{p}^2 v^2 + \Delta^2$$

We actually know from Schrodinger's equation:

$$1 + 1 \rightarrow i\hbar \frac{\partial \psi}{\partial t} = A \left(-i\hbar \frac{\partial \psi}{\partial x} \right)$$

But we actually want:

$$2 + 1 \rightarrow (E^2 = \vec{p}^2 v^2)$$

Consider :

$$\psi = e^{\frac{i}{\hbar}(px - Et)}$$

$$E\psi = Ap\psi$$

And we want

$$E = |p|v$$

2 Dirac Equation

To have both $E = vp$ and $E = -vp$, we will allow A to be a matrix with eigenvalues $= \pm v$. Then, $A = v\sigma^z$ where, $\sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

In this basis, we can write ψ as:

$$\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$$

Then, we get the Dirac equation in 1-D:

$$i\hbar \frac{\partial \psi}{\partial t} = v \left(-i\hbar \frac{\partial}{\partial x} \right) \psi \tag{1}$$

This very nicely gives us the required eigenvalues of energy.

- For $\psi = e^{\frac{i}{\hbar}(px-Et)} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

$$E\psi = vp\psi$$
$$E = vp$$

- For $\psi = e^{\frac{i}{\hbar}(px-Et)} \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

$$E\psi = -vp\psi$$
$$E = -vp$$

Okay. Now we need Δ^2. But LHS is E and not E^2. So RHS eigenvalue should be $\sqrt{p^2v^2 + \Delta^2}$. Let us use:

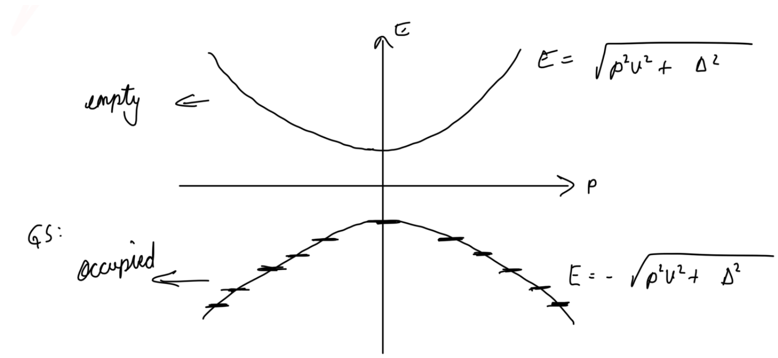
$$i\hbar\frac{\partial\psi}{\partial t} = \left[-i\hbar v\frac{\partial}{\partial x}\sigma^z + \Delta\sigma^x\right]\psi \tag{2}$$

(We could have used σ^y in the above equation as well.)
With:

$$\psi = e^{\frac{i}{\hbar}(px-Et)}(\phi) \tag{3}$$

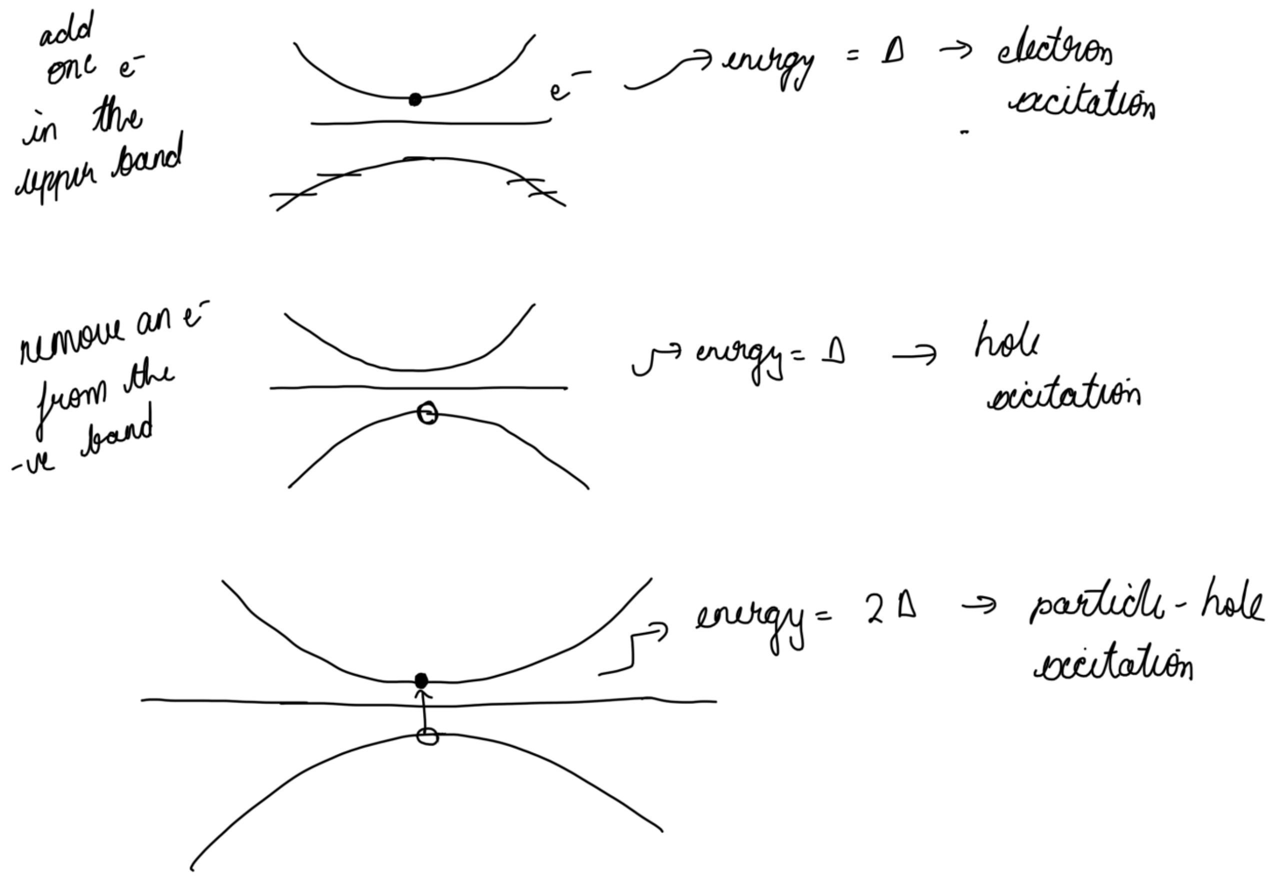
such that: $E\phi = [pv\sigma^z + \Delta\sigma^x]\phi$
The terms within in the brackets in the RHS will give us: $\pm\sqrt{p^2v^2 + \Delta^2}$.
Finally giving us:

$$E = \pm\sqrt{p^2v^2 + \Delta^2}$$



→What are the excited states?

There are different ways in which we can get excited states in this type of dispersion, given that the ground state is the one shown before. We add an electron to the upper band or equivalently we can remove an electron from the lower band.



It turns out that in low-dimensional condensed matter systems, the excitations obey the Dirac equation. →Why would that be the case?

→ Deep revelation about the mathematics involved.

3 Back to Tight-Binding

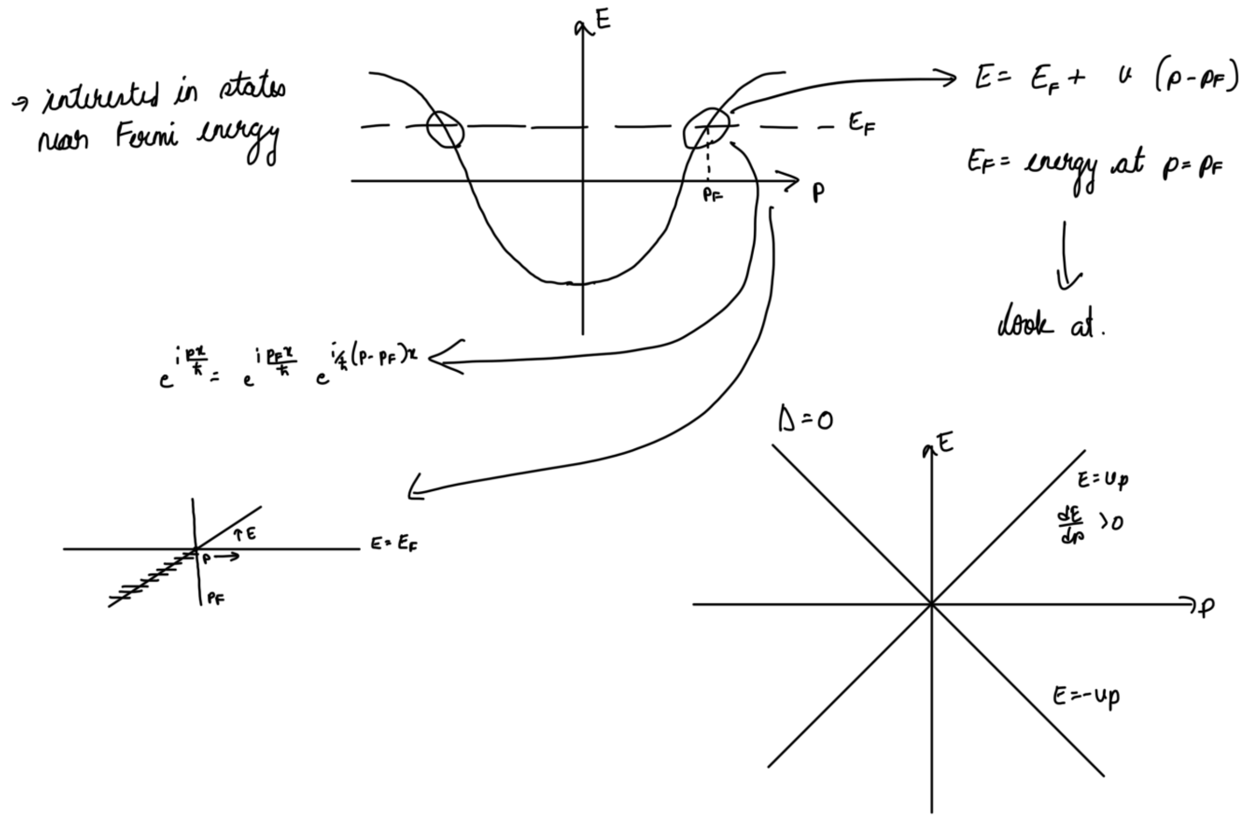
Let us take a look back at the tight-binding model. The Hamiltonian is:

$$H = -\gamma \sum (c^{\dagger}_{n+1} c_{n+1} + h.c.) \tag{4}$$

And the energy spectrum is given by:

$$E = \sum_{-\pi<k<\pi} (-2\gamma cosh(c^{\dagger}_{k} c_{k})) \tag{5}$$

Focusing on the states near the Fermi energy, i.e., states with energy E_F, we notice that the dispersion around that point becomes almost linear. Along with that we can write the travelling wave solutions in a different way by taking out terms of p_F in the exponent.



Then, we can write the wavefunction as:

$$\begin{aligned}\psi &= e^{\frac{i}{\hbar}p_F x}\psi_R(x,t) + e^{\frac{-i}{\hbar}p_F x}\psi_L(x,t) \\ &= e^{\frac{i}{\hbar}(p_F x - E_F t)}\psi_R(x,t) + e^{\frac{-i}{\hbar}(p_F x - E_F t)}\psi_L(x,t)\end{aligned}$$

Here, the two wave functions ψ_R and ψ_L are the rightward and leftward moving waves respectively, with respect to the points $p_F = \pm p_F$ respectively, having energies $E = \pm vp$ respectively as well.

Thus, these two wavefunctions obtained after removal of the Fermi momentum and Fermi energy satisfy the Dirac equation.

- ψ_R:

$$i\hbar\frac{\partial\psi_R}{\partial t} = v\left(-i\hbar\frac{\partial}{\partial x}\right)\psi_R \tag{6}$$

- ψ_L:

$$i\hbar\frac{\partial\psi_L}{\partial t} = -v\left(-i\hbar\frac{\partial}{\partial x}\right)\psi_L \tag{7}$$

In fact, ψ_R and ψ_L constitute two components of a spinor.

$$\psi = \begin{pmatrix}\psi_R \\ \psi_L\end{pmatrix} \to i\hbar\frac{\partial\psi}{\partial t} = v\left(-i\hbar\frac{\partial}{\partial x}\right)\sigma^z\psi$$

$\rightarrow$Here $\Delta = 0$, but when do we get $\Delta \neq 0$ in condensed matter systems?

4 Back to SSH Model

Recall the SSH model from previous lectures. There are two hopping amplitudes which alternate from site to site. This time, let us write the hopping amplitudes differently.

$$\gamma_1 = \gamma - \delta$$
$$\gamma_2 = \gamma + \delta$$

Then, the Hamiltonian will become:

$$H = \gamma\sum(c_n^\dagger c_{n+1} + c_{n+1}^\dagger c_n) - \delta\sum(-1)^n(c_n^\dagger c_{n+1} + c_{n+1}^\dagger c_n) \tag{8}$$

Again, let us take a Fourier transform of the operators:

$$c_n = \frac{1}{\sqrt{L}}\sum_k c_k e^{ikna} \tag{9}$$

$$c_n^\dagger = \frac{1}{\sqrt{L}}\sum_k c_k^\dagger e^{-ikna} \tag{10}$$

And, we get:

$$\begin{aligned} c_n^\dagger c_{n+1} &= \frac{1}{L}\sum_n\sum_k c_k^\dagger e^{-ikna}\sum_{k'} e^{ik'(n+1)a} \\ &= \frac{1}{L}\sum_k c_k^\dagger e^{ika} c_{k'}\delta_{kk'}L \\ &= \sum_k c_k^\dagger c_k e^{ika} \end{aligned}$$

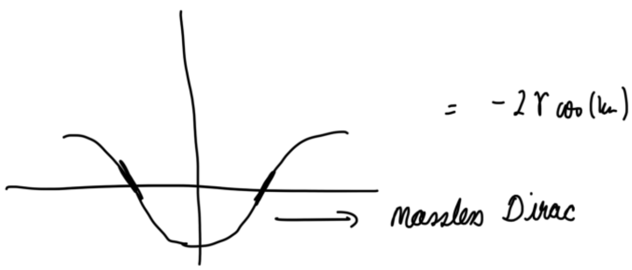
And in the second term in the Hamiltonian, we can write $(-1)^n$ as $e^{i\pi n)}$ to get terms like $c_k^\dagger c_{k+\pi/a}$. Thus, the new Hamiltonian is:

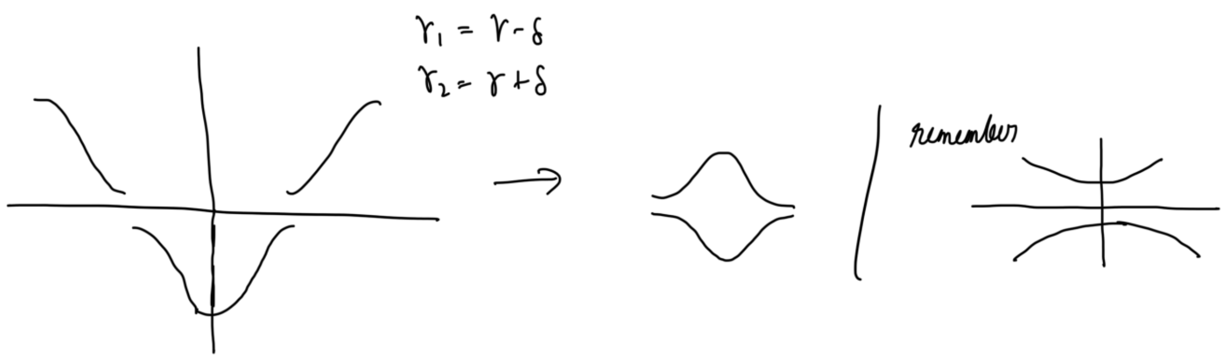
$$\begin{aligned} H &= \sum_{-\pi/a<k<\pi/a} \left[-2\gamma cos(ka) c_k^\dagger c_k - \delta(c_k^\dagger c_{k+\pi/a} + c_{k+\pi/a}^\dagger c_k)\right] \\ &= \sum_{0<k<\pi/a} \begin{pmatrix} c_k^\dagger & c_{k+\pi/a}^\dagger \end{pmatrix} \begin{pmatrix} -2\gamma cos(ka) & -2\gamma \\ -2\gamma & 2\gamma cos(ka) \end{pmatrix} \begin{pmatrix} c_k \\ c_{k+\pi/a} \end{pmatrix} \end{aligned}$$

We know that the energy is given by:

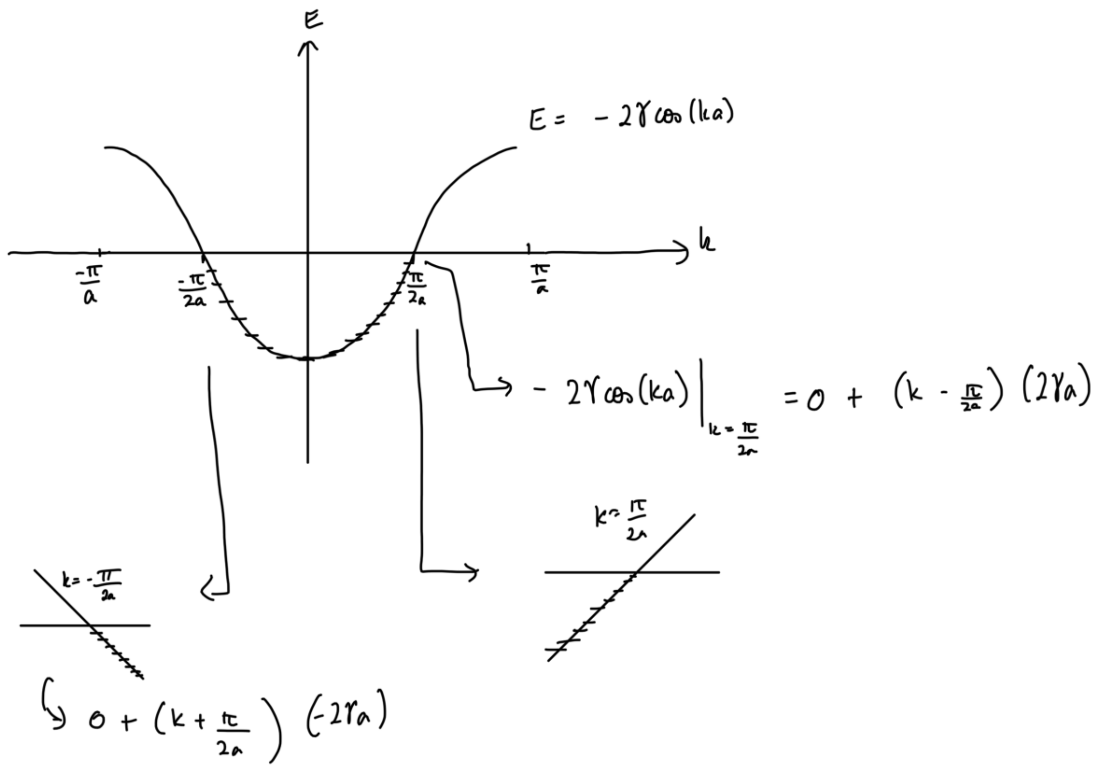
$$E = \pm\sqrt{(2\gamma cos(ka))^2 + (2\delta)^2} \tag{11}$$

Note here that for $\gamma_1 = \gamma_2 = \gamma \implies \delta = 0$, we basically get the massless Dirac equation with a certain type of dispersion shown before. When $\delta \neq 0$, we get a particular dispersion which is what we obtained for the SSH model.





Sticking to the case of massless Dirac equation, let us again expand the energy around the point $E = 0$ or $cos(ka) = 0$.



Since, only states with $E < 0$ are occupied, the Fermi momentum is $k_F = \frac{\pi}{2a}$. Then, for $k_F = \pm\frac{\pi}{2a}$, we get the Hamiltonian as:

$$H = \sum_k \psi^\dagger_{Rk}\psi_{Rk}kv \text{ (about } k_F = \frac{\pi}{2a}) \tag{12}$$

$$H = \sum_k \psi^\dagger_{Lk}\psi_{Lk}k(-v) \text{ (about } k_F = \frac{-\pi}{2a}) \tag{13}$$

Here, $v = 2\gamma a$.

Then, the Hamiltonian becomes:

$$H = \sum_k \left[\psi^\dagger_{Rk}\psi_{Rk}\left(-i\hbar\frac{\partial}{\partial x}\right)v + \psi^\dagger_{Lk}\psi_{Lk}\left(-i\hbar\frac{\partial}{\partial x}\right)(-v) - \delta(\psi^\dagger_R\psi_L + \psi^\dagger_L\psi_R)\right] \tag{14}$$

$$= \sum_k \begin{pmatrix}\psi^\dagger_{Rk} & \psi^\dagger_{Lk}\end{pmatrix}\begin{pmatrix}\left(-i\hbar\frac{\partial}{\partial x}\right)v & -\delta \\ -\delta & \left(-i\hbar\frac{\partial}{\partial x}\right)(-v)\end{pmatrix}\begin{pmatrix}\psi_{Rk} \\ \psi_{Lk}\end{pmatrix} \tag{15}$$

The Dirac equation we get is:

$$\sum_k i\hbar \frac{\partial}{\partial t} \begin{pmatrix} \psi_R \\ \psi_L \end{pmatrix} = \begin{pmatrix} \left(-i\hbar\frac{\partial}{\partial x}\right) v & -\delta \\ -\delta & \left(-i\hbar\frac{\partial}{\partial x}\right)(-v) \end{pmatrix} \begin{pmatrix} \psi_R \\ \psi_L \end{pmatrix} \tag{16}$$

$\rightarrow$Velocity v is related to the hopping amplitude and lattice spacing.
$\rightarrow\delta$ is the effective mass term and it arises from the fact that the hopping amplitude were unequal.