8.511 Problem Set 6

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1 Breakdown of Semiclassical Theory: Zener Tunneling

1.1 Part (a)

QUESTION! If k is complex, the wavefunction is not normalizable?

Even though k is now a general complex number, since $V(x)$ is periodic, the conclusion of Bloch theorem is still valid. Namely, the wavefunction is some function with the period of the lattice, modulated by a spatially linear phase. The only difference is that now this phase becomes complex. Then we can still write

$$\Psi_k(x) = e^{ikx} u_k(x)$$

where $u_k(x)$ is periodic and can be Fourier decomposed as

$$u_k(x) = \sum_G a_{k,G} e^{-iGx}$$

Since k is defined upto G, $a_{k,G}$ can be labeled by $k - G$. In conclusion, the wavefunction labeled by a general k can be expanded as

$$\Psi_k(x) = \sum_G a_{k-G} e^{i(k-G)x}$$

In the vicinity of the zone boundary, the Fourier component $k = G_0/2 + \kappa$ is near degenerate with $k' = -G_0/2 + \kappa$. The coupling between these two states is V_{G_0}. Therefore, the truncated Hamiltonian is

$$\begin{aligned}
H &= \begin{pmatrix} \frac{\hbar^2}{2m}\left(\frac{1}{2}G_0 + \kappa\right)^2 & V_{G_0} \\ V_{G_0}^* & \frac{\hbar^2}{2m}\left(-\frac{1}{2}G_0 + \kappa\right)^2 \end{pmatrix} \\
&\approx E_0 I + \begin{pmatrix} \frac{\hbar^2}{2m} G_0 \kappa & V_{G_0} \\ V_{G_0}^* & -\frac{\hbar^2}{2m} G_0 \kappa \end{pmatrix}
\end{aligned}$$

$E_0 + \varepsilon$ is an eigenvalue. Therefore,

$$\begin{vmatrix} \frac{\hbar^2}{2m} G_0 \kappa - \varepsilon & V_{G_0} \\ V_{G_0}^* & -\frac{\hbar^2}{2m} G_0 \kappa - \varepsilon \end{vmatrix} = 0$$

which simplifies to

$$\begin{aligned}
\kappa^2 &= \frac{\varepsilon^2 - |V_{G_0}|^2}{\left(\frac{\hbar^2 G_0}{2m}\right)^2} \\
&= \frac{2m}{\hbar^2}\left(\frac{\varepsilon^2 - |V_{G_0}|^2}{4E_0}\right)
\end{aligned}$$

1.2 Part (b)

When the electron tunnels, its κ changes with x, such that its total energy is conserved. From A in the valance band to B in the conduction band, the energy gap Δ must be compensated by the electric potential eEd_{AB}. Therefore, the distance between A and B is thus $d_{AB} = \Delta/eE$.

1.3 Part (c)

$$\varepsilon_{\pm}(x) = \sqrt{\frac{\hbar^2}{2m}4E_0\kappa^2(x) + \left(\frac{\Delta}{2}\right)^2}$$

During the tunneling, the change in the energy gap must be compenstated by the electric potential.

$$\varepsilon_+ - \varepsilon_- = \Delta - eE(x_B - x)$$

Therefore,

$$\begin{aligned}\kappa(x) &= \sqrt{\frac{m}{8E_0\hbar^2}\left((\Delta - eE(x_B - x))^2 - \Delta^2\right)} \\ &= \frac{i\Delta}{2\hbar}\sqrt{\frac{m}{2E_0}\left(1 - (1 - (x_B - x)/d_{AB})^2\right)}\end{aligned}$$

Let $x' = x_B - x$.

$$|\kappa(x)| = \frac{\Delta}{2\hbar}\sqrt{\frac{m}{2E_0}\left(1 - (1 - (x'/d_{AB})^2)\right)}$$

Therefore,

$$\begin{aligned}P &= \exp\left(-2\int_A^B |\kappa(x)|dx\right) \\ &= \exp\left(-\frac{\Delta}{\hbar}\sqrt{\frac{m}{2E_0}}\int_0^{d_{AB}}\sqrt{(1 - (1 - (x'/d_{AB})^2))}dx'\right) \\ &= \exp\left(-\frac{\Delta^2}{\hbar eE}\sqrt{\frac{m}{2E_0}}\int_0^1\sqrt{1 - (1 - x'')^2}dx''\right) \\ &= \exp\left(-\frac{\Delta^2}{\hbar eE}\sqrt{\frac{m}{2E_0}}\frac{\pi}{4}\right)\end{aligned}$$

Using $E_0 = \hbar^2G_0^2/8m$ and $G_0 = 2\pi/a$, we get

$$P = \exp(-\pi^2\Delta^2/8E_0eEa)$$

Breakdown of the semiclassical theory happens when $P \ll 1$ no longer holds, i.e., when we no longer have $E \ll \Delta^2/eE_0a$. When E becomes comparable with Δ^2/eE_0a, we must take interband tunneling into account.

2 Rashba Splitting

2.1 Part (a)

$$\begin{aligned}H_{SO} &= -\frac{e\hbar}{4m^2c^2}\boldsymbol{\sigma}\cdot(\mathbf{E}\times\mathbf{p}) \\ &= \frac{e\hbar}{4m^2c^2}\mathbf{E}\cdot(\boldsymbol{\sigma}\times\mathbf{p}) \\ &= \frac{e\hbar^2}{4m^2c^2}E(\boldsymbol{\sigma}\times\mathbf{k})\cdot\mathbf{n}\end{aligned}$$

Comparing with $H_{SO} = \alpha(\boldsymbol{\sigma} \times \mathbf{k}) \cdot \mathbf{n}$, we get

$$\begin{aligned} E &= \frac{4m^2c^2}{e\hbar^2}\alpha \\ &\approx 1.88 \times 10^4 \text{ V/Å} \end{aligned}$$

It is larger than the estimated actual electric field by 7 orders of magnitude.

2.2 Part (b)

Let $\mathbf{n} = \hat{\mathbf{z}}$. Then $H_{SO} = \alpha(\boldsymbol{\sigma} \times \mathbf{k}) \cdot \mathbf{n} = \alpha(k_y\sigma_x - k_x\sigma_y)$. $|\mathbf{k}, \uparrow\rangle$ is coupled with $|\mathbf{k}, \downarrow\rangle$.

$$\begin{aligned} H_{SO}|\mathbf{k},\uparrow\rangle &= \alpha(k_y - ik_x)|\mathbf{k},\downarrow\rangle \\ H_{SO}|\mathbf{k},\downarrow\rangle &= \alpha(k_y + ik_x)|\mathbf{k},\uparrow\rangle \end{aligned}$$

Therefore,

$$\begin{aligned} \langle\mathbf{k},\uparrow|H_{SO}|\mathbf{k},\uparrow\rangle &= \langle\mathbf{k},\downarrow|H_{SO}|\mathbf{k},\downarrow\rangle = 0 \\ \langle\mathbf{k},\uparrow|H_{SO}|\mathbf{k},\downarrow\rangle &= \langle\mathbf{k},\downarrow|H_{SO}|\mathbf{k},\uparrow\rangle^* = \alpha(k_y + ik_x) \end{aligned}$$

Moreover, different $\mathbf{k}$ states do not couple because $\mathbf{k}$ is a good quantum number of H_{SO}. Then the two-level Hamiltonian is

$$H = \begin{pmatrix} \frac{\hbar^2\mathbf{k}^2}{2m} & \alpha(k_y + ik_x) \\ \alpha(k_y - ik_x) & \frac{\hbar^2\mathbf{k}^2}{2m} \end{pmatrix}$$

The band structure is

$$E_\pm(\mathbf{k}) = \frac{\hbar^2\mathbf{k^2}}{2m} \pm \alpha|\mathbf{k}|$$

which is plotted in Fig.1

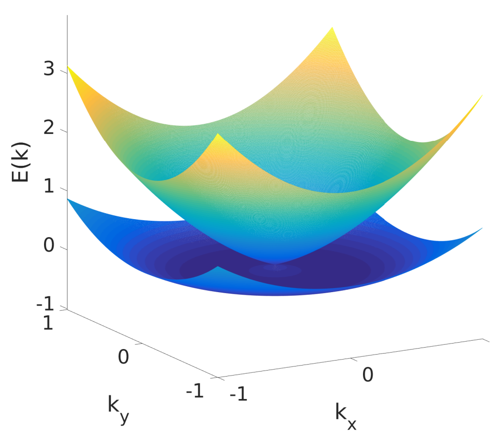

Figure 1: Band splitting by spin-orbit coupling

Let $\mathbf{k} = (k, \theta)$.

$$H = \begin{pmatrix} \frac{\hbar^2k^2}{2m} & i\alpha ke^{-i\theta} \\ -i\alpha ke^{i\theta} & \frac{\hbar^2k^2}{2m} \end{pmatrix}$$

The eigenvector for band $E_-(\mathbf{k})$ is

$$|\Psi_{\mathbf{k}}^-\rangle = \frac{1}{\sqrt{2}}(1, ie^{i\theta})^T = \frac{1}{\sqrt{2}}|\mathbf{k}\rangle(|\uparrow\rangle + ie^{i\theta}|\downarrow\rangle)$$

The eigenvector for band $E_+(\mathbf{k})$ is

$$|\Psi_{\mathbf{k}}^+\rangle = \frac{1}{\sqrt{2}}(1, -ie^{i\theta})^T = \frac{1}{\sqrt{2}}|\mathbf{k}\rangle(|\uparrow\rangle - ie^{i\theta}|\downarrow\rangle)$$

2.3 Part (c)

Since $E_\pm(\mathbf{k})$ depends only on $|\mathbf{k}|$, the Fermi surfaces are two concentric circles. E_+ corresponds to the smaller radius and E_- corresponds to the larger radius. This is shown in Fig.2.

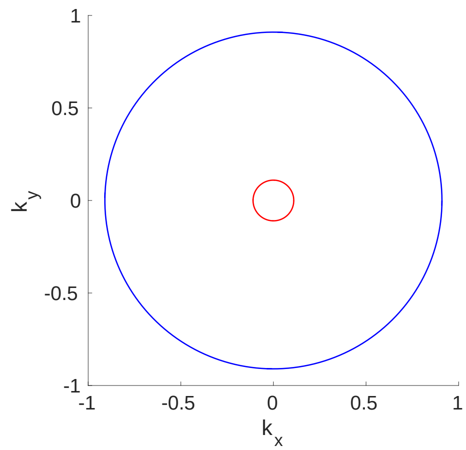

Figure 2: The Fermi surfaces

$$\langle\Psi_{\mathbf{k}}^-|\sigma_x|\Psi_{\mathbf{k}}^-\rangle = \frac{1}{2}(1, -ie^{-i\theta})\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ ie^{i\theta} \end{pmatrix} = -\sin\theta$$
$$\langle\Psi_{\mathbf{k}}^-|\sigma_y|\Psi_{\mathbf{k}}^-\rangle = \frac{1}{2}(1, -ie^{-i\theta})\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} 1 \\ ie^{i\theta} \end{pmatrix} = \cos\theta$$
$$\langle\Psi_{\mathbf{k}}^-|\sigma_z|\Psi_{\mathbf{k}}^-\rangle = \frac{1}{2}(1, -ie^{-i\theta})\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 1 \\ ie^{i\theta} \end{pmatrix} = 0$$
$$\langle\Psi_{\mathbf{k}}^+|\sigma_x|\Psi_{\mathbf{k}}^+\rangle = \frac{1}{2}(1, ie^{-i\theta})\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ -ie^{i\theta} \end{pmatrix} = \sin\theta$$
$$\langle\Psi_{\mathbf{k}}^+|\sigma_y|\Psi_{\mathbf{k}}^+\rangle = \frac{1}{2}(1, ie^{-i\theta})\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} 1 \\ -ie^{i\theta} \end{pmatrix} = -\cos\theta$$
$$\langle\Psi_{\mathbf{k}}^+|\sigma_z|\Psi_{\mathbf{k}}^+\rangle = \frac{1}{2}(1, ie^{-i\theta})\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 1 \\ -ie^{i\theta} \end{pmatrix} = 0$$

Therefore,

$$\langle\mathbf{S}(\mathbf{k})\rangle|_{|\mathbf{k}|=k_F^-} = -\frac{1}{2}\hat{\mathbf{k}} \times \hat{\mathbf{z}}$$
$$\langle\mathbf{S}(\mathbf{k})\rangle|_{|\mathbf{k}|=k_F^+} = \frac{1}{2}\hat{\mathbf{k}} \times \hat{\mathbf{z}}$$

On the inner circle (E_+), spin direction rotates clockwise. On the outer circle (E_-), spin direction rotates counterclockwise. This is shown in Fig.2.