8.511 Problem Set 6

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1 Breakdown of Semiclassical Theory: Zener Tunneling

1.1 Part (a)

Since the potential $V(x)$ is perodic, we can expand it into discrete Fourier components,

$$V(x) = \sum_G V_G e^{iGx}$$

The Fourier transform of $\Psi(x)$ is (suppose the system is finite, so the integral is replaced by a summation)

$$\Psi(x) = \sum_k a_k e^{ikx}$$

where in general k is complex. Plugging these expansions into the Schrödinger equation, we have

$$\sum_k \frac{\hbar^2 k^2}{2m} a_k e^{ikx} + \sum_k \sum_G V_G a_{k-G} e^{ikx} = \sum_k E a_k e^{ikx}$$

We can see that only those k differ by G are coupled.

$$\frac{\hbar^2 k^2}{2m} a_k + \sum_G V_G a_{k-G} = E_k a_k$$

The corresponding wavefunction can be labelled as Ψ_k, where $\mathrm{Re}(k)$ is taken within the first Brillouin zone.

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

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)

Inside the band, $\kappa(x)$ is real. During the tunneling, $\kappa(x)$ is imaginary. At the start and the end of tunneling, κ must reach its critical value, which is 0. This gives $(eEx_A)^2 = (eEx_B)^2 = |V_{G_0}|^2$. Therefore,

$$\begin{aligned}x_A &= -\frac{|V_{G_0}|}{eE} = -\frac{\Delta}{2eE} \\ x_B &= \frac{|V_{G_0}|}{eE} = \frac{\Delta}{2eE} \\ d = x_B - x_A &= \frac{2|V_{G_0}|}{eE} = \frac{\Delta}{eE}\end{aligned}$$

1.3 Part (c)

Let $\varepsilon(x) = eEx$. Then during the tunneling,

$$|\kappa(x)| = \sqrt{\frac{2m}{4E_0\hbar^2}\left(|V_{G_0}|^2 - (eE)^2x^2\right)}$$

Therefore,

$$\begin{aligned}\int_{x_A}^{x_B} |\kappa(x)|dx &= \sqrt{\frac{2m}{4E_0\hbar^2}}\int_{-|V_{G_0}|/eE}^{|V_{G_0}|/eE} \sqrt{|V_{G_0}|^2 - (eE)^2x^2}dx \\ &= \sqrt{\frac{m}{2E_0\hbar^2}}\frac{|V_{G_0}|^2}{eE}\int_{-1}^{1}\sqrt{1-x'^2}dx' \\ &= \sqrt{\frac{m}{2E_0\hbar^2}}\frac{\pi\Delta^2}{8eE}\end{aligned}$$

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

$$\begin{aligned}P &= \exp\left(-2\int_{x_A}^{x_B}|\kappa(x)|dx\right) \\ &= \exp\left(-\frac{\pi^2\Delta^2}{8E_0 eEa}\right)\end{aligned}$$

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

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

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

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

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

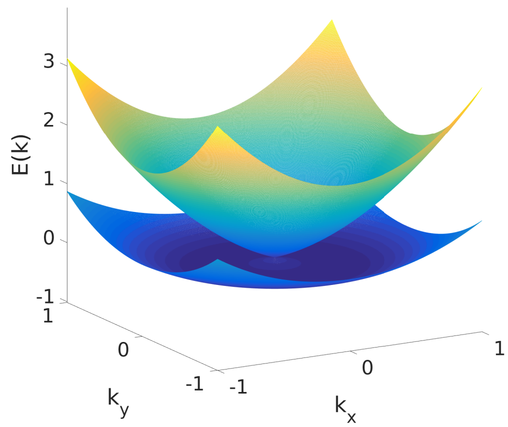

Figure 1: Band splitting by spin-orbit coupling

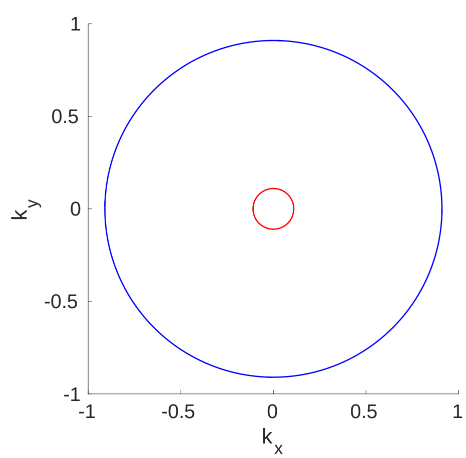

Figure 2: The Fermi surfaces

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.

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

Therefore,

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

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