《量子信息基础》2022.3.22 随堂作业：

1. Derive the following equation of Bloch function in periodic potentials from the time-independent Schrodinger equation:

$$\frac{d^2u}{dx^2}+2ik\frac{du}{dx}+\left(\frac{2m}{\hbar^2}(E-V)-k^2\right)u=0$$

将布洛赫波的形式

$$\psi(x)=e^{ikx}u(x)$$

代入定态薛定谔方程

$$\frac{d^2\psi}{dx^2}+\frac{2m}{\hbar^2}\big(E-V(x)\big)\psi=0$$

的左面，得到

$$\begin{aligned}\frac{d^2\psi}{dx^2}+\frac{2m}{\hbar^2}(E-V)\psi &= \frac{d^2e^{ikx}u}{dx^2}+\frac{2m}{\hbar^2}(E-V)e^{ikx}u \\ &= \frac{d}{dx}\left(ike^{ikx}u+e^{ikx}\frac{du}{dx}\right)+\frac{2m}{\hbar^2}(E-V)e^{ikx}u \\ &= -k^2e^{ikx}u+2ike^{ikx}\frac{du}{dx}+e^{ikx}\frac{d^2u}{dx^2}+\frac{2m}{\hbar^2}(E-V)e^{ikx}u \\ &= e^{ikx}\left[\frac{d^2u}{dx^2}+2ik\frac{du}{dx}+\left(\frac{2m}{\hbar^2}(E-V)-k^2\right)u\right]=0\end{aligned}$$

所以

$$\frac{d^2u}{dx^2}+2ik\frac{du}{dx}+\left(\frac{2m}{\hbar^2}(E-V)-k^2\right)u=0$$

推导正确给 20 分

2. (Text book* Problem 7.8)
Let the two “good” unperturbed states be

$$\psi_\pm^0=\alpha_\pm\psi_a^0+\beta_\pm\psi_b^0$$

where $\alpha_\pm$ and $\beta_\pm$ are determined (up to normalization) by Equation 7.27 (or Equation 7.29). Show explicitly that
(a) $\psi_\pm^0$ are orthogonal ($\langle\psi_+^0|\psi_-^0\rangle=0$);

$$\begin{aligned}\langle\psi_+^0|\psi_-^0\rangle &= \langle\alpha_+\psi_a^0+\beta_+\psi_b^0|\alpha_-\psi_a^0+\beta_-\psi_b^0\rangle \\ &= \alpha_+^*\alpha_-\langle\psi_a^0|\psi_a^0\rangle+\alpha_+^*\beta_-\langle\psi_a^0|\psi_b^0\rangle+\beta_+^*\alpha_-\langle\psi_b^0|\psi_a^0\rangle+\beta_+^*\beta_-\langle\psi_a^0|\psi_a^0\rangle \\ &= \alpha_+^*\alpha_-+\beta_+^*\beta_-\end{aligned}$$

由 7.27 可得

$$\beta_\pm=\frac{\alpha_\pm\left(E_\pm^1-W_{aa}\right)}{W_{ab}}$$

$$\langle\psi_+^0|\psi_-^0\rangle=\alpha_+^*\alpha_-+\frac{\alpha_+^*\alpha_-}{|W_{ab}|^2}\left[E_+^1E_-^1-W_{ab}(E_+^1+E_-^1)+|W_{ab}|^2\right]$$

由于

$$E_{\pm}^{1}=\frac{1}{2}\left[W_{aa}+W_{bb}\pm\sqrt{(W_{aa}-W_{bb})^2+4|W_{ab}|^2}\right]$$

代入可得

$$\langle\psi_{+}^{0}|\psi_{-}^{0}\rangle=0$$

推导正确给 20 分

(b) $\langle\psi_{+}^{0}|H'|\psi_{-}^{0}\rangle=0$;

$$\begin{aligned}\langle\psi_{+}^{0}|H'|\psi_{-}^{0}\rangle&=[\alpha_{+}^{*}\quad\beta_{+}^{*}]\begin{bmatrix}W_{aa}&W_{ab}\\W_{ba}&W_{bb}\end{bmatrix}\begin{bmatrix}\alpha_{-}\\\beta_{-}\end{bmatrix}\\&=\alpha_{+}^{*}\alpha_{-}W_{aa}+\alpha_{+}^{*}\beta_{-}W_{ab}+\beta_{+}^{*}\alpha_{-}W_{ba}+\beta_{+}^{*}\beta_{-}W_{bb}\\&=\alpha_{+}^{*}\alpha_{-}W_{aa}+\alpha_{+}^{*}\alpha_{-}(E_{-}^{1}-W_{aa})+\alpha_{+}^{*}\alpha_{-}(E_{+}^{1}-W_{aa})\\&-\alpha_{+}^{*}\alpha_{-}W_{bb}=\alpha_{+}^{*}\alpha_{-}(E_{+}^{1}+E_{-}^{1}-W_{aa}-W_{bb})=0\end{aligned}$$

推导正确给 15 分

(c) $\langle\psi_{\pm}^{0}|H'|\psi_{\pm}^{0}\rangle=E_{\pm}^{1}$, where $E_{\pm}^{1}$ given by Equation 7.33.

$$\begin{aligned}\langle\psi_{\pm}^{0}|H'|\psi_{\pm}^{0}\rangle&=[\alpha_{\pm}^{*}\quad\beta_{\pm}^{*}]\begin{bmatrix}W_{aa}&W_{ab}\\W_{ba}&W_{bb}\end{bmatrix}\begin{bmatrix}\alpha_{\pm}\\\beta_{\pm}\end{bmatrix}\\&=|\alpha_{\pm}|^2W_{aa}+\alpha_{\pm}^{*}\beta_{\pm}W_{ab}+\beta_{\pm}^{*}\alpha_{\pm}W_{ba}+|\beta_{\pm}|^2W_{bb}\end{aligned}$$

$$\begin{aligned}\beta_{\pm}W_{ab}&=\alpha_{\pm}(E_{\pm}^{1}-W_{aa})\\\alpha_{\pm}W_{ba}&=\beta_{\pm}(E_{\pm}^{1}-W_{bb})\end{aligned}$$

$$\langle\psi_{\pm}^{0}|H'|\psi_{\pm}^{0}\rangle=\left(|\alpha_{\pm}|^2+|\beta_{\pm}|^2\right)E_{\pm}^{1}=E_{\pm}^{1}$$

推导正确给 15 分

3. Considering we have free electron gas in a rectangular area in two dimension, derive the Fermi energy and the density of energy states in two dimension. *Note: the Fermi-energy formula written on the text book was derived in three dimension. You need follow the same procedure but the result will be slightly different comparing to the three dimension case.*

The wavefunction should have the form of

$$\begin{aligned}X(x)&=A_x\sin(k_xx)+B_x\cos(k_xx)\\Y(y)&=A_y\sin(k_yy)+B_y\cos(k_yy)\end{aligned}$$

where

$$k_x\equiv\frac{\sqrt{2mE_x}}{\hbar},k_y\equiv\frac{\sqrt{2mE_y}}{\hbar}$$

Considering the following boundary conditions held

$$X(0) = Y(0) = 0, \; X(l_x) = Y(l_y) = 0$$

The solutions for wavefunctions are

$$\psi_{n_x,n_y,n_z} = \sqrt{\frac{4}{l_x l_y}} \sin\left(\frac{n_x \pi}{l_x} x\right) \sin\left(\frac{n_y \pi}{l_y} y\right)$$

The area in the k-space every state would occupy

$$\frac{\pi^2}{l_x l_y} = \frac{\pi^2}{S}$$

For $k_F \leq \frac{\sqrt{2mE_F}}{\hbar}$

$$n(E_F) = N = 2 \cdot \frac{1}{4} \cdot \pi k_F^2 \cdot \frac{S}{\pi^2} = \frac{S}{2\pi}\left(\frac{2mE_F}{\hbar^2}\right) = \frac{SmE_F}{\pi\hbar^2}$$

So

$$E_F = \frac{\pi N \hbar^2}{mS}$$

$$\rho(E) = \frac{dn(E)}{SdE} = \frac{m}{\pi\hbar^2}$$

如果没考虑自旋，会多一个 1/2 因子，也算对

推导正确和给出正确答案给 30 分

* David J. Griffiths, and Darrell F. Schroeter, Introduction to Quantum Mechanics (3rd Edition), Cambridge University Press (2018).