《量子信息基础》第三章第二部分：

1. Derive the following equation of Bloch function in periodic potentials from the time-independent Schrodinger equation:
$$\frac{d^2u}{dx^2}+2ik\frac{du}{dx}+\left(\frac{2m}{\hbar^2}(E-V)-k^2\right)u=0$$

将布洛赫定理
$$\psi(x)=e^{ikx}u(x)$$
代入周期性方势阱的薛定谔方程
$$\frac{d^2\psi}{dx^2}+\frac{2m}{\hbar^2}\big(E-V(x)\big)\psi=0$$
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

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

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

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

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

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

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

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

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

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

3. (Text book* Problem 7.1)
   Suppose we put a delta-function bump in the center of the infinite square well:
   $$H' = \alpha\delta(x - a/2)$$
   where α is a constant.
   (a) Find the first-order correction to the allowed energies. Explain why the energies are not perturbed for even *n*.

$$\psi_n^0 = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a} x\right)$$

$$E_n^1 = \langle \psi_n^0 | H' | \psi_n^0 \rangle = \frac{2\alpha}{a} \int_0^a \sin^2\left(\frac{n\pi}{a} x\right) \delta\left(x - \frac{a}{2}\right) dx = \frac{2\alpha}{a} \sin^2\left(\frac{n\pi}{2}\right)$$

For even *n*

$$E_n^1 = 0$$

(b) Find the first three nonzero terms in the expansion (Equation 7.13) of the correction to the ground state, ψ_1^1.

$$\psi_1^1 = \sum_{m=2}^{\infty} \frac{\langle \psi_m^0 | H' | \psi_1^0 \rangle}{E_1^0 - E_m^0} \psi_m^0$$

$$\langle \psi_m^0 | H' | \psi_1^0 \rangle = \frac{2\alpha}{a} \int_0^a \sin\left(\frac{m\pi}{a}x\right) \sin\left(\frac{\pi}{a}x\right) \delta\left(x - \frac{a}{2}\right) dx = \frac{2\alpha}{a} \sin\left(\frac{m\pi}{2}\right)$$

$$E_1^0 - E_m^0 = \frac{\hbar^2\pi^2}{2Ma^2}(1 - m^2)$$

The first three non-zero terms are m = 3, 5, 7.

$$\psi_1^1 = \frac{2\alpha}{a}\frac{2Ma^2}{\hbar^2\pi^2}\left[\frac{1}{8}\sqrt{\frac{2}{a}}\sin\left(\frac{3\pi}{a}x\right) - \frac{1}{24}\sqrt{\frac{2}{a}}\sin\left(\frac{5\pi}{a}x\right) + \frac{1}{48}\sqrt{\frac{2}{a}}\sin\left(\frac{7\pi}{a}x\right)\cdots\right]$$

$$= \frac{M\alpha}{\hbar^2\pi^2}\sqrt{\frac{a}{2}}\left[\sin\left(\frac{3\pi}{a}x\right) - \frac{1}{3}\sin\left(\frac{5\pi}{a}x\right) + \frac{1}{6}\sin\left(\frac{7\pi}{a}x\right)\cdots\right]$$

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