First-order perturbation theory

The Hamiltonian $\hat{H}$ for an electron (with mass m_0 and momentum operator $\hat{p}$) in one spatial dimension exposed to a potential $V(x)$ is given by

$$\hat{H} = \frac{\hat{p}^2}{2m_0} + V. \tag{1}$$

We assume that the potential is periodic with periodicity L, i.e., $V(x + nL) = V(x)$ for any integer n. Felix Bloch has shown that the wave function ψ for such a periodic potential can be written in the form

$$\psi(x) = e^{ikx} u_k(x) \tag{2}$$

as a product of a plane wave with a momentum-dependent function $u_k(x)$ that has the same periodicity as the potential, i.e.,

$$u_k(x + nL) = u_k(x). \tag{3}$$

The wave vector k is related to the momentum eigenvalue p by $p = \hbar k$, where $\hbar$ is the reduced Planck's constant. Assume that the solution of the Hamiltonian (1) for k=0 is known and given by the normalized wave function $\psi_0 = u_0$ with energy eigenvalue E_0. The solution ψ_0 is non-degenerate.

<u>**Problems:**</u>

1. By plugging the Bloch wave function (2) into the Hamiltonian (1), show that the function u_k must satisfy the equation

$$\left[\frac{\hat{p}^2}{2m_0} + \frac{\hbar}{m_0} k\hat{p} + \frac{\hbar^2 k^2}{2m_0} + V\right] u_k(x) = E(k)\, u_k(x), \tag{4}$$

   where $E(k)$ is the energy eigenvalue of the Hamiltonian (1) for the momentum $p = \hbar k$.

2. Since we know the solution ψ_0 with energy E_0 for the case of vanishing momentum k=0, treat the k-dependent terms as a small perturbation. Within first-order perturbation theory and keeping terms to second order in k, calculate the energy $E(k)$ for small values of k. Use the definition $P = \langle \psi_0 | \hat{p} | \psi_0 \rangle$ for the momentum matrix element.

Note 1: Treat everything in one dimension to keep the notation simple. (This works just as well in three dimensions.)
Note 2: I might also add that this problem has no practical applications. In practice, the matrix element P is usually zero and one must go to second order degenerate perturbation theory to get useful results.

Solution:

1. Plugging the Bloch wave function (2) into the Hamiltonian (1) yields the equation

$$H\psi(x) = He^{ikx}u_k(x) = \frac{\hat{p}^2}{2m_0}e^{ikx}u_k(x) + Ve^{ikx}u_k(x). \tag{1}$$

The momentum operator is $\hat{p} = -i\hbar d/dx$. The product rule for differentiation yields

$$\begin{aligned}\hat{p}e^{ikx}u_k(x) = -i\hbar\frac{d}{dx}\left[e^{ikx}u_k(x)\right] &= \\ &= -i\hbar\left[ike^{ikx}u_k(x) + e^{ikx}\frac{d}{dx}u_k(x)\right] = -i\hbar e^{ikx}\left[iku_k(x) + \frac{d}{dx}u_k(x)\right]. \end{aligned}\tag{2}$$

$$\begin{aligned}\hat{p}^2e^{ikx}u_k(x) = \hat{p}\left\{-i\hbar e^{ikx}\left[iku_k(x) + \frac{d}{dx}u_k(x)\right]\right\} &= \\ = -i\hbar\frac{d}{dx}\left\{-i\hbar e^{ikx}\left[iku_k(x) + \frac{d}{dx}u_k(x)\right]\right\} &= \\ = -\hbar^2\frac{d}{dx}\left\{e^{ikx}\left[iku_k(x) + \frac{d}{dx}u_k(x)\right]\right\} &= \\ = -\hbar^2\left\{ike^{ikx}\left[iku_k(x) + \frac{d}{dx}u_k(x)\right] + e^{ikx}\left[ik\frac{d}{dx}u_k(x) + \frac{d^2}{dx^2}u_k(x)\right]\right\} &= \\ = -\hbar^2e^{ikx}\left[-k^2u_k(x) + 2ik\frac{d}{dx}u_k(x) + \frac{d^2}{dx^2}u_k(x)\right] &= \\ = -\hbar^2e^{ikx}\left[-k^2 + 2ik\frac{d}{dx} + \frac{d^2}{dx^2}\right]u_k(x). \end{aligned}\tag{3}$$

The Schrödinger equation therefore takes the form

$$H\psi(x) = He^{ikx}u_k(x) = -\frac{\hbar^2}{2m_0}e^{ikx}\left[-k^2 + 2ik\frac{d}{dx} + \frac{d^2}{dx^2}\right]u_k(x) + Ve^{ikx}u_k(x) = E(k)\,e^{ikx}u_k(x), \tag{4}$$

where $E(k)$ is the energy corresponding to the momentum $p = \hbar k$. If we cancel the complex exponential on both sides, we see that the function $u_k(x)$ must satisfy the equation

$$\left[\frac{\hbar^2k^2}{2m_0} - \frac{ik\hbar^2}{m_0}\frac{d}{dx} - \frac{\hbar^2}{2m_0}\frac{d^2}{dx^2} + V\right]u_k(x) = E(k)\,u_k(x). \tag{5}$$

Given the definition $\hat{p} = -i\hbar d/dx$ of the momentum operator, this is equivalent to

$$\left[\frac{\hat{p}^2}{2m_0} + \frac{\hbar}{m_0}k\hat{p} + \frac{\hbar^2k^2}{2m_0} + V\right]u_k(x) = E(k)\,u_k(x). \tag{6}$$

2. Within first-order perturbation theory with a perturbation Hamiltonian $\hat{H}'$ and a non-degenerate solution ψ_0 of the unperturbed Hamiltonian, the energy correction is $\Delta E = \langle\psi_0|H'|\psi_0\rangle$. In our case

$$\Delta E(k) = \left\langle\psi_0\left|\frac{\hbar}{m_0}k\hat{p} + \frac{\hbar^2k^2}{2m_0}\right|\psi_0\right\rangle = \frac{\hbar kP}{m_0} + \frac{\hbar^2k^2}{2m_0}. \tag{7}$$

The energy eigenvalue of the Hamiltonian is therefore

$$E(k) = E_0 + \frac{\hbar^2k^2}{2m_0} + \frac{\hbar kP}{m_0}. \tag{8}$$