1. Band structure

A fairly good model of electrons in a crystalline solid is of independent particles confined to a macroscopic box, moving in the presence of a periodic potential of positively charged ions. We will study a one-dimensional version of this problem. The corresponding single-electron Hamiltonian is \( H = \frac{p^2}{2m} + V_{\text{ions}}(x) \). The potential satisfies \( V_{\text{ions}}(x+a) = V_{\text{ions}}(x) \), and the box is taken to have periodic boundaries. For simple (e.g., alkali) metals, to zeroth order one can even simply ignore the periodic potential, approximating electron waves by plane-waves, with energy spectrum \( E^0_k = \frac{\hbar^2 k^2}{2m} \). [30pts:5+5+5+5+5+5]

(a) Use non-degenerate perturbation theory to compute the correction to this quadratic spectrum to second-order and the eigenfunctions to first-order in the periodic potential \( V_{\text{ions}}(x) \). Write down your answer for a generic periodic potential \( V_{\text{ions}}(x) \), expressing it in terms of the Fourier coefficients \( V_{Q_n} \) of the periodic potential; \( Q_n = nQ_1 \) is the \( n \)th Fourier wavevector, with \( n \) running over integers and \( Q_1 \) is the smallest non-zero wavevector characterizing \( V_{\text{ions}}(x) \). (What is \( Q_1 \) in terms of \( a \)?) You need not evaluate the infinite sum, but simplify the expression as much as possible.

(b) Specialize this result to the potential \( V_{\text{ions}}(x) = V_1 \cos(Q_1 x) \). We will work with this specific form of the potential for the rest of the problem.

(c) By examining your expression above, note that for some values of \( k \), the above nondegenerate perturbation theory breaks down. Find these special values \( k^* \) for which this breakdown happens.

Using the properties of the unperturbed, free particle spectrum, \( E^0_k \), and the nature of the perturbing Hamiltonian, explain why the breakdown takes place.

(d) Sketch the resulting \( E_k \), indicating the location of special \( k \) points.

(e) Apply a lowest order (1st order in \( V_{\text{ions}} \)) degenerate perturbation theory to compute the perturbed energies and eigenstates right at these special \( k \) points, where the non-degenerate perturbation theory breaks down.

Hint: There are only two such \( k \) points.

(f) Now that you know exactly what happens right at these special \( k \) points and far away from them (where nondegenerate perturbation theory is valid), make an educated guess of what happens to the spectrum around the special \( k \) points, sketching it for all values of \( k \).

Hint: The spectrum must be continuous away from these special values of \( k \).

2. Let’s try to solve by variational methods the ground state of an infinite well [30pts:10+10+10]

\[
V(x) = \begin{cases} 
0 & \text{for} |x| < a \\
\infty & \text{for} |x| > a 
\end{cases}
\]

(a) Find the exact ground state function and ground state energy.

(b) Assuming the variational ansatz \( \psi(x) = a^2 - x^2 \) compute the ground state energy.

(c) Show that a much better result can be obtained by the trial wave function \( \psi(x) = |a|^\lambda - |x|^\lambda \)
3. Consider a one-dimensional potential well of a given shape $U(x)$ with the characteristic depth $U_0$ and width $a$ which obey the following inequality
\[
\frac{\hbar^2}{ma^2} \gg U_0
\]
where $m$ is the mass of a quantum particle moving in this potential. (Such a well is called shallow.) Using the variational method, find [30pts:10+10+10]:

(a) An expression for the ground state energy of the particle
(b) Compare the ground state energy with $U_0$. Is the ground state a bound one?
(c) What is the characteristic localization length of the ground state wave function? Compare it is with $a$.

4. Perturbed harmonic oscillator transitions [30pts:15+15]

(a) Consider a charged particle in the ground state of a 1D harmonic oscillator potential $V(x) = \frac{1}{2}m\omega^2x^2$, this time perturbed at time $t = 0$ by a weak oscillating electric field $E\cos\omega e t$. Calculate the transition rate out of the ground state at time $t$. What is the asymptotic, long-time rate?
(b) Repeat the above analysis if instead of an electric field, the perturbation is a periodically modulated oscillator frequency, i.e., $\omega \rightarrow \omega(t) = \omega + \omega_0 \cos\omega e t$, where the amplitude of frequency modulation is weak, $\omega_0 \ll \omega$. 