Homework Assignment 1

Due before class Monday, February 8.

1. Consider how the de Broglie’s suggestion might explain some properties of the hydrogen atom.
   a. Show that the assumption
   \[ p = mυ = \frac{h}{\lambda} \]
   and the ‘quantization condition’ that the length of a circular orbit be an integer multiple of the length of the electron wavelength (that is: \( n\lambda = 2\pi r \), where \( r \) is the radius of the orbit and \( n \) an integer) imply that only discrete orbits are allowed.
   b. Calculate the total energy (kinetic plus potential) of the electron in each orbit characterized by \( n \).

Hint: In part a find two equations describing the balance between the centrifugal and the Coulomb (centripetal) force. Solve for the radius \( r \) and for the angular velocity \( \omega \). Now, in b insert these expressions into the formulae for the kinetic and potential energy.

2. Let’s consider the tunneling problem (Notes, page 7) with the potential barrier:

\[
V(z) = \begin{cases} 
0 & \text{for } z \leq 0 \\
V > 0 & \text{for } 0 < z < L \\
0 & \text{for } z \geq L \end{cases}
\]

Write the wavefunction as:

\[
\psi(z) = \begin{cases} 
Ae^{ikz} + Be^{-ikz} & \text{for } z \leq 0 \\
Ce^{\kappa z} + De^{-\kappa z} & \text{for } 0 < z < L \\
Fe^{ikz} & \text{for } z \geq L 
\end{cases}
\]

with \( k = (2mE)^{1/2}/\hbar, \kappa = [2m(V - E)]^{1/2}/\hbar \).
   a. Write the system of four equations expressing the continuity of the wavefunction and its derivative at \( z = 0 \)
and at $z = L$.

**b.** Find the transmission coefficient, $T = |F|^2/|A|^2$. There’s no need to solve the full system. Be creative. Hint: Multiply the equation expressing continuity of $\psi$ at $z = 0$ by $ik$ and add and subtract it from the equation expressing continuity of the derivatives at $z = 0$. Do a similar thing with the other two equations (by multiplying one by $\kappa$). Now it should be relatively easy to solve for $F$ in terms of $A$ alone. This gives you $T$.

3. From the Schrödinger equation derive the continuity equation:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot S = 0,$$

where $\rho = |\Psi|^2$ is the ‘probability density’ and $S = \frac{i\hbar}{2m}[\Psi \nabla \Psi^* - \Psi^* \nabla \Psi]$ is the ‘probability density current’.

4. The Wentzel-Kramers-Brillouin (WKB) approximation to solve the Schrödinger equation consists in writing the solution of the time-independent problem:

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

as

$$\psi(x) \approx \frac{1}{k^{1/2}} \exp \left\{ i \int x k(x') \, dx' \right\},$$

where $k(x) = \{2m[E - V(x)]\}^{1/2}/\hbar$. This is a good approximation if the potential $V(x)$ varies slowly (that is, it does not change much compared to the electron energy $E$ when $x$ varies over several de Broglie wavelengths). If $E - V(x) < 0$, the WKB wavefunction becomes

$$\psi(x) \approx \frac{1}{k^{1/2}} \exp \left\{ - \int x \kappa(x') \, dx' \right\},$$

where now $\kappa(x) = \{2m[V(x) - E]\}^{1/2}/\hbar$.

Let’s now ignore the factor $k^{-1/2}$ (which simply ensures continuity of probability current). Consider now the
previous tunneling problem (problem 2) and identify the WKB approximation to the transmission coefficient as:

\[
T_{WKB} = |\psi(L)|^2 = \exp\left\{ -2 \int_0^L \kappa(x') \, dx' \right\} .
\] (1)

Compare \(T_{WKB}\) with the 'exact' transmission coefficient \(T\) of the previous tunneling problem (problem 2) in the limit in which \(\kappa L >> 1\).

5. Calculate the matrix element between two wavefunctions of the form

\[
\psi(k, r) = \frac{1}{V^{1/2}} e^{i k \cdot r} \quad \text{and} \quad \psi(k', r) = \frac{1}{V^{1/2}} e^{i k' \cdot r},
\]

and the perturbation potentials of the form:

a. \(H \propto e^{i q \cdot r}\)

b. \(H \propto \delta(r)\)

c. \(H \propto |r|^{-2}\)

d. \(H \propto e^{-|r|}/r_0\)

Polar coordinates are useful in c and d.

6. Show in detail the equivalence between the two formulations of Bloch theorem:

\[
\psi(k, r + R_l) = e^{i k \cdot R_l} \psi(k, r) ,
\] (2)

and:

\[
\psi(k, r) = e^{i k \cdot r} u_k(r) ,
\] (3)

where \(u_k(r)\) is periodic:

\[
u_k(r + R_l) = u_k(r).
\]

7. a. Find the reciprocal lattice vectors of the fcc lattice. As fundamental translation vectors use

\[
a = \frac{a}{2}(\hat{x} + \hat{y}) , \quad b = \frac{a}{2}(\hat{y} + \hat{z}) , \quad c = \frac{a}{2}(\hat{z} + \hat{x}).
\]
b. Find the volume of the BZ.