HW#5 —Phys622—Spring 1998
Due Friday, March 6, 1998
Turn in at or before beginning of class.

Prof. Ted Jacobson
Room 4117, (301)405-6020
jacobson@physics.umd.edu

1. Show that, as $|\psi\rangle$ varies over all quantum states, the expectation value of the energy $\langle\psi|H|\psi\rangle$ takes on its minimum value when $|\psi\rangle$ is the ground state of H. [3 *points*]

2. Show that for a particle of mass m in one dimension, the expectation value of the energy can be written as

$$\langle\psi|H|\psi\rangle = \int dx \, \left\{ \frac{\hbar^2}{2m} \left(\frac{d\psi}{dx}\right)^* \left(\frac{d\psi}{dx}\right) + V\psi^*\psi \right\}. \tag{1}$$

Note that the kinetic energy contribution to the integrand is positive everywhere. [1 *point*]

3. Consider a one-dimensional potential well of a given (arbitrary) shape $V(x)$, such that

$$\int V(x)\, dx < 0. \tag{2}$$

Suppose the overall characteristic depth V_0 and width a of the potential obey the following inequality:

$$V_0 \ll \hbar^2/ma^2, \tag{3}$$

where m is the mass of a quantum particle moving in this potential. (Such a well is called *shallow*. Roughly speaking, it is a well for which the depth of the well is much less than the uncertainty in kinetic energy of a particle confined to the vicinity of the well.) In one dimension a shallow well always has a bound state, but the wave function of this state is very spread out compared to the well. In this problem you will show this in two different ways, both rough approximations. [5+5=10 *points*]

(a) Replace the arbitrary shallow potential $V(x)$ by a delta function with the same value of $\int V(x)\, dx$ and find the energy E_0 and the wave function $\psi_0(x)$ of the bound state. (See HW#3.10.)
Compare E_0 with the depth of the potential V_0 and the width of the wave function $\psi_0(x)$ with the width of the potential a.

(b) Suppose the wave function ψ is nonzero and slowly varying in some region of size $\lambda \gg a$, so that $\psi \sim \lambda^{-1/2}$ and $d\psi/dx \sim \lambda^{-3/2}$. Use (1) to see how $\langle\psi|H|\psi\rangle$ depends on λ, and minimize this expression to find an estimate for the size and energy of the ground state. Compare with your delta function result from the previous part.

4. *Adapted from Physics Qualifier, August 1990 and 1980, Problem II-1.*

In the semiconductor device called the field-effect transistor, electrons are held against an oxidized surface of the semiconductor by an electric field $\mathcal{E}$ and cannot escape through the surface. Thus, the electrons experience the following potential: [2+2+2+6=12 *points*]

$$V(x) = \begin{cases} \infty, & x < 0, \\ e\mathcal{E}x, & x > 0. \end{cases} \tag{4}$$

(a) Taking into account only the one-dimensional motion perpendicular to the surface, write the Schrödinger equation for the wave function $\psi(x)$ of an electron in the potential (4).

(b) The Airy function $\mathrm{Ai}(x)$ satisfies the equation $[d^2/dx^2 - x]\mathrm{Ai}(x) = 0$ and vanishes when $x \to +\infty$: $\mathrm{Ai(x)} \to x^{-1/4} \exp\left(-\frac{2}{3}x^{3/2}\right)$. By suitable change of variables, cast the Schrödinger equation for $\psi(x)$ into the form of an Airy equation.

(c) The Airy function $\mathrm{Ai}(x)$ has its zeros at $x_0 = -2.338, -4.008, -5.521$, etc. Obtain an expression for the bound state energies in terms of $\hbar$, the electron mass m, the electric force $e\mathcal{E}$, and x_0, by imposing appropriate boundary conditions on the wave function obtained from the Airy equation.

(d) Estimate the ground state energy by minimizing $\langle\psi|H|\psi\rangle$ with respect to variations of the parameter a in the trial wave function $\psi(x) = N(a)xe^{-ax}$ (where $N(a)$ is a normalization factor. Compare your result with the exact result from the previous part.

5. Consider a "double square well potential", with wells of depth V_0 and width a, separated by a distance b. Suppose the depth and width are fixed and great enough that so that several bound states exist. This problem is to be done by *strictly qualitative* reasoning (no calculation allowed). [6+4+2=12 *points*]

(a) Sketch the ground and first excited state wave functions for the three cases $b = 0$, $b \approx a$, and $b \gg a$.

(b) Qualitatively, how do the corresponding energies E_0 and E_1 vary as b goes from 0 to ∞? Sketch $E_0(b)$ and $E_1(b)$ on the same graph.

(c) Is there a force of attraction or repulsion between the two wells when a particle is in the ground state? How about in the first excited state?

6. Problem 3.12, Schwabl (*half an oscillator*) [3 *points*]

7. *Adapted from Physics Qualifier, Fall 1985, Problem II-5.*

Let us consider a particle in one dimension subject to a periodic potential: [3+7+10=20 *points*]

$$V(x+a) = V(x). \tag{5}$$

(a) Define the translation operator T_a by $(T_a\psi)(x) = \psi(x+a)$. Show that T_a is unitary and commutes with the particle Hamiltonian.

(b) Since T_a commutes with the Hamiltonian, the energy eigenbasis can be assumed to be eigenstates of T_a as well,

$$(T_a\psi_\delta)(x) = e^{i\delta}\psi_\delta(x). \tag{6}$$

(We showed this in class for hermitian operators, but since a unitary operator is the exponential of i times a hermitian operator, the result holds for unitary operators as well.)

i. Explain why the eigenvalues of T_a are phases $e^{i\delta}$.

ii. In other books or articles you will come across the statement that the energy eigenstates of the Hamiltonian can be assumed to have the form:

$$\psi_k(x) = e^{ikx}u_k(x), \tag{7}$$

where $u_k(x)$ is a periodic function of x: $u_k(x+a) = u_k(x)$, and k is a parameter, called quasimomentum, that labels the eigenstates and their eigenenergies $E(k)$. (Eq. (7) is called *Bloch's theorem* in quantum mechanics and *Floquet's theorem* in mathematics.) Derive this from the fact that we can use the T_a-eigenstates ψ_δ (6), and find the relation between δ and k.

iii. Which momenta does the state ψ_δ contain? In other words, which wave vectors occur in its Fourier expansion?

(c) Suppose the potential consists of periodically spaced delta-functions:

$$V(x) = \lambda \sum_n \delta(x - na) \tag{8}$$

(the so-called *Dirac comb*).

For this potential, write down the Schrödinger equation for the eigenfunctions ψ_δ and obtain an equation that determines a relation between the quasimomentum k and energy E (the so-called *dispersion relation*). Study this equation graphically and show that the energy E may take values only within certain ranges, called the *energy bands*, and may not take value within other ranges, called the *energy gaps*. Consider both positive and negative values for λ and E.