Massachusetts Institute of Technology
Physics Department

Physics 8.322 **Spring 2007**
Quantum Theory II **February 26, 2007**

Assignment 4

Due March 9, 2007, at the end of the day

Announcements

- Problem Sets can be downloaded from http://web.mit.edu/8.321/

Reading topics for this period

- Continuing discussion of perturbation theory and its applications to classic problems in atomic physics.
- The variational principle and applications.
- The semiclassical method, also known as the WKB-approximation (Wenzel, Kramers, Brioullin). The importance of this method has been increasing over the years. I will have to supplement the material in the texts with additional notes and photocopies from other sources. [For some reason, Sakurai does not treat it *at all*! – a major defect.]

Reading Recommendations 4

- Sakurai: Perturbation theory and applications to hydrogen: §5.1 – 5.3; Variational Principle: §5.4. Sakurai gives an extensive discussion of geometric phases in Supplement I, page 464 – 480.
- Gottfried and Yan, the WKB approximation is discussed in §4.5, and the semi-classical approximation to the sum-over-histories is discussed in §2.8. The adiabatic approximation and geometric phases are discussed briefly in §7.7.
- Landau and Lifschitz give a famous discussion of both the semiclassical method and the adiabatic approximation in §xxx, but don't expect to be able to follow all of it. I can't.
- Griffiths gives a straightforward treatment of WKB (including a pedestrian derivation of the connection formulas) in §8. His treatment of the adiabatic approximation and geometric phases in §10 is similar to Sakurai's.

Problem Set 4

Topics covered in the problems

- The variational method
- The adiabatic approximation

Problems

1. **A linear potential**

   Use the variational method to estimate the lowest energy eigenvalue for a particle that moves in a potential, $V(r) = kr$. Compare your estimate with the exact result. [Make an intelligent *ansatz* for the wavefunction. The better your estimate, the more points you will score!]

2. **Constraints**

   Suppose E_0 is the ground state energy of a quantum system. Now suppose a constraint is imposed on the system, $F[\psi] = 0$, where F is some functional of the state ψ. Show that the ground state energy of the constrained system is greater than or equal to E_0.

3. **Adding a basis state**

   In class I discussed an approximation method based on "partial diagonalization". The aim of this problem is for you to fill in the steps in the various derivations.

   Let H be a Hamiltonian in a Hilbert space $\mathcal{H}$ with discrete eigenvalues. Let $\{\phi_j, j = 1, 2, ...n\}$ be a set of n *orthonormal* states in $\mathcal{H}$ spanning a subspace $\mathfrak{h}_n$. Note that the states $\{\phi_j\}$ *are not* eigenstates of H. They are just a convenient set of basis states. Often they are taken to something very simple, like harmonic oscillator eigenstates.

   Diagonalize H in $\mathfrak{h}_n$, giving a set of eigenvectors $\{\tilde{\phi}_j, j = 1, n\}$ and eigenvalues that we order in increasing energy: $e_1^{(n)} < e_2^{(n)} < e_3^{(n)} ... < e_n^{(n)}$. Assume, for simplicity, that none are equal (no degeneracies).

   (a) Prove that $e_1^{(n)}$ is the best variational upper limit on the lowest eigenvalue of H that can be obtained from any state in $\mathfrak{h}_n$

   (b) Now add another eigenvector, ϕ_{n+1}, orthogonal to the others $\{\phi_j, j = 1, 2, ...n\}$. These eigenvectors span $\mathfrak{h}_{n+1}$. Label the eigenvalues of H in $\mathfrak{h}_{n+1}$ by $\{e_j^{(n+1)}, j = 1, 2, ...n + 1\}$, again increasing in energy. Assume that none of the matrix elements, $H_{j,n+1} \equiv \langle\tilde{\phi}_j|H|\phi_{n+1}\rangle$ vanishes. Show that the old and new eigenvalues are *interlaced*. Specifically,

   $$e_1^{(n+1)} < e_1^{(n)} < e_2^{(n+1)} < e_2^{(n)} < e_3^{(n+1)} ... < e_j^{(n)} < e_{j+1}^{(n+1)} ... < e_n^{(n)} < e_{n+1}^{(n+1)}$$

(c) Part (c) has been deleted.

4. **The minimax principle**

The variational principle states that the ground state energy is the minimum of the Hamiltonian functional over all states $|\psi\rangle$ in the Hilbert space, $\mathcal{H}$,

$$E_0 = \min_{|\psi\rangle \in \mathcal{H}} \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}$$

and the state on which E reaches its minimum is the ground state, $|\psi_0\rangle$. Prove the following extension:

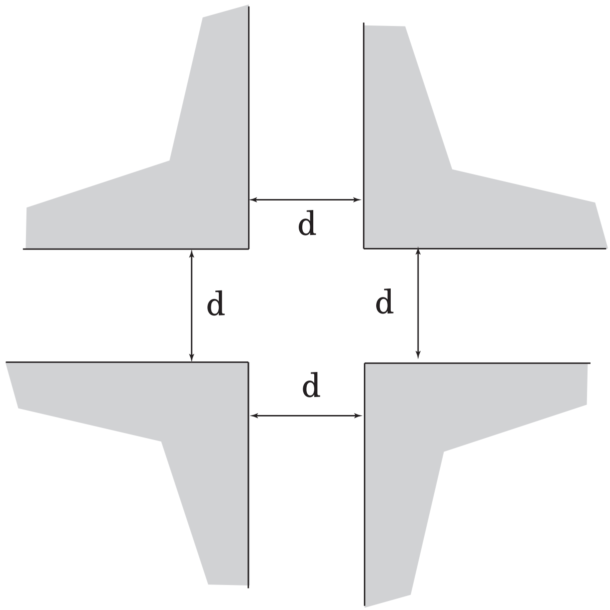
Let $\{|\phi_1\rangle, |\phi_2\rangle ... |\phi_n\rangle\}$ be any set of n linearly independent states in $\mathcal{H}$. Minimize the Hamiltonian functional over all states *orthogonal* to $\{|\phi_1\rangle, |\phi_2\rangle ... |\phi_n\rangle\}$,

$$E_n[\phi_1, \phi_2 ... \phi_n] = \min_{|\psi\rangle \in \mathcal{H},\, \langle\phi_j|\psi\rangle = 0,\, \forall j} \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} \tag{1}$$

Then the energy of the n^{th} excited state of H is the *maximum* of E_n over the $\{|\phi_j\rangle\}$'s:

$$E_n = \max_{\{\phi_j\}} E_n[\phi_1, \phi_2 ... \phi_n]$$

and, given the set $\{\phi_i\}$ maximising E_n, the state ψ saturating eq. (1) is the n^{th} excited state.



5. **The quantum crossroads prize**

   The student, or group (collaborate if you like), who submits the best bound will win a $50 gift certificate at the Harvard/MIT Coop!

   Consider the two dimensional domain shown in the Figure. The constant width "arms" continue out to infinity.

   (a) What is the threshold energy for propagating (continuum) states?

   (b) Are there other thresholds? What does the spectrum of continuum states look like?

   (c) Show that this system has a bound (*ie.* normalizable, non-propagating) state.

   (d) Find the best variational estimate of the energy of the bound state you can. Please do not use more than *two* variational parameters (to keep the work under control).

   Answer: The best estimate I know of is $E \leq 0.66 \times \pi^2$, where I've set $\hbar^2/2md^2 = 1$. If you are interested in this and related problems, see R. L. Jaffe and J. Goldstone, Phys. Rev. **B45**, 14100 (1992).

6. **WKB approximation to the transition amplitude**

   Scattering from a potential, $V(x)$, in one dimension is described in terms of reflection and transmission amplitudes, $R(E)$ and $T(E)$, according to the parameterization of the wave function,

$$\psi(x) = \begin{cases} e^{ikx} + R(E)e^{-ikx} & \text{as } x \to -\infty \\ T(E)e^{ikx} & \text{as } x \to \infty \end{cases}$$

(where $k = \sqrt{2mE/\hbar^2}$), corresponding to a plane wave incident from the left.

Assume that $V(x) \to 0$ as $x \to \pm\infty$ and that $V(x)$ is smooth. When the energy E is much greater than the maximum of the potential, the WKB conditions are satisfied for all x, and $|T(E)| \approx 1$. So $T(E) = e^{2i\delta(E)}$.

(a) Write an expression for the phase, $\delta(E)$ in the WKB approximation. Your result should be an integral over x.

(b) There are some simple potentials for which the phase can be calculated exactly. One such case is $V(x) = -\frac{\hbar^2}{ma^2}\,\text{sech}^2(x/a)$. The resulting Schrödinger equation,

$$-\frac{d^2}{dz^2}\psi - 2\,\text{sech}^2 z\psi = (ka)^2\psi$$

can be solved exactly with the result that $\delta(E) = 1/(ka)$. Compare the WKB result (which you may want to compute numerically) with the exact one. Is it valid where you expect it to be?

7. **WKB approximation to the density of states**

Consider a deep, smooth potential in one dimension. It has many bound states. According to the WKB (Bohr-Sommerfeld) quantization condition,

$$\int_{x_1(E)}^{x_2(E)} dx\sqrt{2m(E - V(x))} = (N(E) + \frac{1}{2})\pi\hbar$$

where x_1 and x_2 are the turning points of the classical motion. Show that

$$\frac{dN}{dE} = \frac{T(E)}{\hbar}$$

where $T(E)$ is the period of the classical motion with energy E.