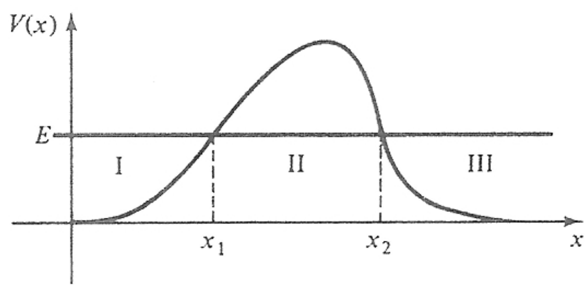
Physics 125b – Problem Set 9 – Due Jan 22, 2008

Version 2 – Jan 19, 2008

This problem set focuses on the WKB and variational approximation techniques – Shankar Chapter 16 and Lecture Notes 11.
Version 2: Important typos and algebraic errors in Problem 1, minor (obvious) typos in Problem 5 fixed. Add comment in Problem 2 that you may assume orbital angular momentum vanishes.

Many basic problems in QM can be found in textbooks – there are only so many solvable elementary problems out there. Please refrain from using solutions from other textbooks. Obviously, you will learn more and develop better intuition for QM by solving the problems yourself. We are happy to provide hints to get you through the tricky parts of a problem, but you *must* learn to set up and solve these problems from scratch by yourself.

1. Let's consider the WKB approximation for tunneling through a potential barrier. We of course do not consider a step potential barrier, but rather one that has smooth enough edges to ensure the $|d\lambda/dx| \ll 1$ requirement is satisfied everywhere except possibly for transition regions at the two edges of the barrier. See the figure below.



Potential step for WKB tunneling problem.

We will derive the tunneling probability. We assume $E < \max[V(x)]$ so that there are classical turning points x_1 and x_2 and a region II that is not classically accessible.

(a) Assume a particle incident from the left side so that the solutions in regions I (incident + reflected waves), II (tunneling region), and III (transmitted wave) are

$$\psi_I(x) = \frac{1}{\sqrt{p(x)}} \exp\left(-\frac{i}{\hbar}\int_x^{x_1} dx'\, p(x') - i\,\frac{\pi}{4}\right) + \frac{r}{\sqrt{p(x)}} \exp\left(\frac{i}{\hbar}\int_x^{x_1} dx'\, p(x') + i\,\frac{\pi}{4}\right) \tag{1}$$

$$\psi_{II}(x) = \frac{\alpha}{\sqrt{\kappa(x)}} \exp\left(\frac{1}{\hbar}\int_{x_1}^{x} dx'\kappa(x')\right) + \frac{\beta}{\sqrt{\kappa(x)}} \exp\left(-\frac{1}{\hbar}\int_{x_1}^{x} dx'\kappa(x')\right) \tag{2}$$

$$\psi_{III}(x) = \frac{t}{\sqrt{p(x)}} \exp\left(\frac{i}{\hbar}\int_{x_2}^{x} dx'\, p(x') + i\,\frac{\pi}{4}\right) \tag{3}$$

where

$$p(x) = \sqrt{2\,m\,(E - V(x))} \qquad\qquad \kappa(x) = \sqrt{2\,m\,(V(x) - E)} \tag{4}$$

where r, α, β, and t are coefficients to be determined. (We neglect overall normalization, hence there is no coefficient to be determined for the first term in ψ_I.) We make a linear approximation to the potential in the transition regions near x_1 and x_2, so we know that the full solution to the Schrödinger Equation in these regions will be Airy functions. (Why does this explain our inclusion of $\pi/4$ in the arguments of the complex exponentials outside the transition regions?) Using the asymptotic forms of the Airy functions to connect across the transition regions, show that the matching conditions between ψ_I and ψ_{II} and between ψ_{II} and ψ_{III} are

$$i(1 - r) = -2\,\beta \qquad 1 + r = \alpha \qquad i\,t = 2\,\alpha\,e^{a} \qquad t = \beta\,e^{-a} \tag{5}$$

$$\text{with} \qquad a = \frac{1}{\hbar}\int_{x_1}^{x_2} dx'\kappa(x') \tag{6}$$

Why are the forms we have assumed for the incident, reflected, and transmitted waves correct (*i.e.*, show they have the correct sign of the dependence of the phase on position)?

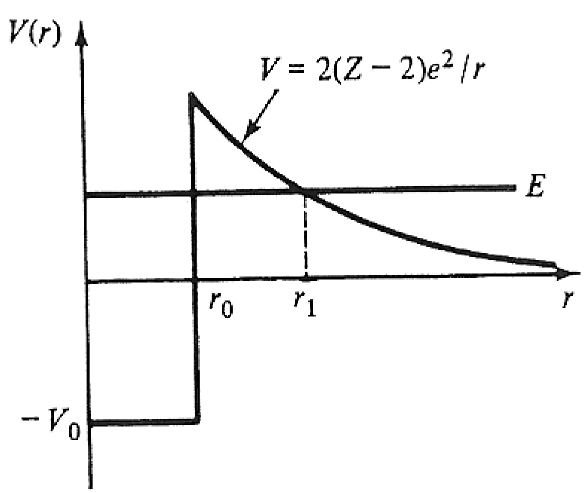
(b) Calculate the transmission probability based on the above. Explain why you may make an approximation that reduces the transmission probability to

$$T = e^{-2\,a} \tag{7}$$

2. A primary mode of decay for radioactive nuclei is through the process of α emission. A model for this process envisions the α particle bound to the nuclear by a square well potential in radius. Outside the well, the α particle is repelled from the residual nucleus by the potential barrier

$$V(r) = \frac{2(Z-2)e^2}{r} \equiv \frac{A}{r} \tag{8}$$

The original radioactive nucleus has charge Ze while the α particle has charge $2e$. See the figure below for a sketch of the full potential.



Nuclear potential for α decay.

(a) Use the WKB approximation as derived in Problem 1 to calculate the transmission probability T of the nuclear barrier for α decay in terms of the velocity $v = \sqrt{2E/m}$ and the dimensionless ratio $\cos W \equiv \sqrt{r_0/r_1}$. You may assume the orbital angular momentum vanishes so that the problem may be treated as one-dimensional in r and Problem 1 applies directly. What form does T assume in the limit $r_0 \to 0$?

(b) Assuming that the α particle "bounces" freely between the walls of the well with speed $\sim 10^9$ cm/s and that the radius of the nucleus is $\sim 10^{-12}$ cm, one obtains that the α particle strikes the barrier at the rate $\sim 10^{21}$/s. It follows that the probability of tunneling through the barrier per second is $P = 10^{21}\,T$, where T is the transmission probability calculated above, and that the mean lifetime of the nucleus is $\tau = 1/P = 10^{21}/T$ sec. Use your answer to part (a) for T and the following expression for the nuclear radius

$$r_0 = 2 \times 10^{-13}\, Z^{1/3}\,\text{cm} \tag{9}$$

to estimate the mean lifetime for uranium α decay. Look up the true value for comparison.

3. Do a web search to find an application of the WKB method (not necessarily related to quantum mechanics) and describe it, briefly. It must be beyond a simple textbook-level application.

4. Consider the anharmonic oscillator,

$$V(x) = \frac{1}{2}\,k\,x^2 + \alpha\,x^4 \tag{10}$$

Use the variational technique to estimate the ground state and first excited state energies. You will have to choose appropriate trial wavefunctions (Hint: look at the standard SHO wavefunctions.)

5. In the lecture notes, we considered the use of the variational technique to obtain an upper limit on the ground-state energy. We will now prove a more powerful version of this method, called the Hylleraas-Undheim Theorem.

Consider a set of n orthonormalized kets, $\{|\chi_i^{(n)}\rangle\}$. One may construct a trial state from them

$$|\psi\rangle = \sum_{i=0}^{n-1} c_i |\chi_i^{(n)}\rangle \tag{11}$$

where we require the c_i to be real for simplicity. Consider the standard energy functional

$$E[\psi] = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{\sum_{i,j=0}^{n-1} c_i\, c_j\, \langle\chi_i^{(n)}|H|\chi_j^{(n)}\rangle}{\sum_{i=0}^{n-1} c_i^2} \tag{12}$$

Let us minimize $E[\psi]$ with respect to the n undetermined coefficients $\{c_i\}$, $\frac{\partial E}{\partial c_i} = 0$ for every c_i. We obtain the set of n equations

$$\sum_{j=0}^{n-1} \left(\langle\chi_i^{(n)}|H|\chi_j^{(n)}\rangle - E\,\delta_{ij}\right) c_j = 0 \qquad i = 0, 1, \ldots, n-1 \tag{13}$$

where the E are undetermined. This is just the eigenvalue-eigenvector equation for H in the subspace spanned by the $\{|\chi_i^{(n)}\rangle\}$,

$$\left(H^{(n)} - E\, I^{(n)}\right) \vec{c} = 0 \tag{14}$$

where $H^{(n)}$ is the matrix representation of the Hamiltonian H in the vector subspace spanned by the $\{\chi_i^{(n)}\}$ and $I^{(n)}$ is the identity matrix in that subspace. Nontrivial solutions $\vec{c}$ are obtained if the determinant of the matrix operator vanishes,

$$|H^{(n)} - E\, I^{(n)}| = 0 \tag{15}$$

There will be in general n solutions to this equation, $\{E_i^{(n)}\}$, $i = 0, \cdots, n-1$, where the ${}^{(n)}$ superscript indicates that the E_i are estimates based on a subspace of dimension n. (We assume we have sorted them in increasing order, $E_0^{(n)} \leq E_1^{(n)} \leq \cdots \leq E_{n-1}^{(n)}$.) The corresponding eigenvectors $\{\vec{c}_i^{\,(n)}\}$ yield n wavefunctions $|\psi_i^{(n)}\rangle$ with $|\psi_i^{(n)}\rangle = \sum_{j=0}^{n-1} (\vec{c}_i^{\,(n)})_j |\chi_j\rangle$.

The Hylleraas-Undheim theorem states two things:

(a) If one compares the estimates obtained with n trial wavefunctions and the estimate obtained by adding one additional orthonormalized trial wavefunction χ_{n+1}, one finds that the new energy estimates are interleaved with the old ones,

$$E_0^{(n+1} \leq E_0^{(n)} \leq E_1^{(n+1)} \leq E_1^{(n)} \cdots \leq E_{n-1}^{(n+1)} \leq E_{n-1}^{(n)} \leq E_n^{(n+1)} \tag{16}$$

(b) The eigenvalues $\{E_i^{(n)}\}$ are upper limits to the corresponding excited states. That is, if E_i is the true energy of the ith excited state (with $i = 0$ being the ground state), then $E_i \leq E_i^{(n)}$.

The result is a successive approximation scheme in which one can obtain a first upper-bound estimate for the nth excited state energy by solving the eigenvalue-eigenvector problem for H in a subspace spanned by n orthonormalized states, and in which the estimate improves monotonically downward toward the true nth excited state energy as one expands the subspace in which the eigenvalue-eigenvector problem for H is solved. One can see why this would be useful: the estimates for the nth excited state energy march monotonically downward, so one can get a reasonable estimate of how good one's approximation is by monitoring the change in the estimate as the subspace size is expanded.

This is a far more interesting constraint than the one we obtained in class for a first excited state trial wavefunction ψ_1 that is orthonormal to the ground state wavefunction ψ_0, which was $E[\psi_1] \geq E_1 - \delta_0(E_1 - E_0)$ with $\delta_0 = 1 - |\langle\psi_0\,|\phi_0\rangle|^2$ where ϕ_0 is the true ground-state wavefunction. There, $E[\psi_1]$ was simply not necessarily an upper bound to E_1.

So, after all that exposition, we would like you to prove two things:

(a) Prove the interleaving aspect; *i.e.*, that when the subspace is expanded by one dimension from n to $n+1$, the new estimates lie between the old estimates. Do this as follows:

   i. Use the $\{|\psi_i^{(n)}\rangle\}$ that result from diagonalization of the n-dimensional subspace as the first n basis functions for the $n+1$ subspace, rather than using the $\{|\chi_i^{(n)}\rangle\}$. Explain why this change allows no less general a choice of the $(n+1)$st state that will be added. Write the matrix $H^{(n+1)} - E\, I^{(n+1)}$; the choice of basis will result in a relatively simple form, which you should write out in terms of the $\{E_i^{(n)}\}$ and the n unknown matrix elements of H between the newly added state $|\chi_n^{(n+1)}\rangle$ and the $\{|\psi_i^{(n)}\rangle\}$.

ii. Denote the determinant of $H^{(n+1)} - E\, I^{(n+1)}$ by $f^{(n+1)}(E)$; it will be an order $n+1$ polynomial in E. One may evaluate this polynomial at the $\{E_i^{(n)}\}$ obtained from the n-dimensional subspace. Show that $f^{(n+1)}(E_i^{(n)})$ alternates sign between successive values of i, obtain the $E \to +\infty$ and $E \to -\infty$ limiting behavior, and use these results to show that the zeroes of $f^{(n+1)}(E)$ – which will of course be the $\{E_i^{(n+1)}\}$ – are interleaved between the $\{E_i^{(n)}\}$.

(b) Assuming the interleaving aspect is true, show that $E_i^{(n)} \geq E_i$; *i.e.*, that the estimate for E_i is always an upper limit to E_i. Hint: what is the limit on how much the subspace can be expanded?