

Massachusetts Institute of Technology  
Physics Department

Physics 8.322  
Quantum Theory II  
*Assignment 5*

Spring 2007  
March 5, 2007

DUE MARCH 16, 2007, AT THE END OF THE DAY

**Announcements**

- There will be a “make-up” lecture this Friday, March 9, 11-12:30, in 4-159 (note the room).
- The usual lecture on Monday, March 12, is cancelled.
- Several sets of supplementary notes have appeared on the 8.322 website. Their titles are:
  - Perturbation Theory Summary
  - Notes on WKB Connection Formulas
  - Summary of WKB Connection Formulas
  - Notes on WKB Approximation for Reflection above a Barrier and The Transition Amplitude in the Adiabatic Approximation

**Reading topics for this period**

- 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.]
- The adiabatic approximation. I may get to this topic at the end of the week. So I list some reading, though the lectures on the subject will likely begin next week.

**Reading Recommendations 5**

- On the WKB approximation
  - Supplementary notes on the connection formulas for the WKB approximation and on the problem of reflection above a barrier.
  - 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.
  - Landau and Lifschitz give a famous discussion of both the semiclassical method and the adiabatic approximation, 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.
- Adiabatic approximation
  - Sakurai pays little attention to the adiabatic theorem, but has a good discussion of Berry's phase in Supplement I.
  - Griffith's treatment of the adiabatic approximation (§10) is similar to Sakurai's.
  - Landau and Lifschitz §41 introduces the adiabatic approximation and §53 describes the transition amplitude in the adiabatic approximation.

**Problem Set 4****Topics covered in the problems**

- More on perturbation theory and the variational approximation
- The WKB approximation

**Problems****1. Variational principle versus perturbation theory**

Consider the one dimensional harmonic oscillator subject to a perturbation

$$H = a^\dagger a + \frac{1}{2} + \alpha(2a^2 + 2a^{\dagger 2} + a^{\dagger 2} a^2)$$

Note: I've set  $\hbar\omega = 1$ . The exact form of the perturbation is chosen for simplicity rather than physical relevance.

- (a) Calculate the ground state energy shift to second order in  $\alpha$ . Note only the  $n = 0$  and  $n = 2$  oscillator states enter.

- (b) Diagonalize  $H$  in the truncated space spanned by the  $n = 0$  and  $n = 2$  states to obtain a bound on the ground state energy.
- (c) Is there a region of  $\alpha$  for which the variational estimate is more accurate than perturbation theory?

Note the implications of this: If you calculate  $\langle 2|V|0\rangle$  you can get an estimate of the ground state energy shift from second order perturbation theory. If you're willing to calculate one more number,  $\langle 2|V|2\rangle$ , and diagonalize a  $2 \times 2$  matrix, you can sometimes do better.

## 2. Variational principle for the anharmonic oscillator

Consider the Hamiltonian

$$H = \frac{1}{2}p^2 + \frac{1}{2}x^2 + \lambda x^{2n} = H_0 + \Delta H$$

The object of this problem is to find the best variational upper limit to the ground state energy with a Gaussian ansatz

$$\psi_\beta(x) = N(\beta)e^{-\frac{1}{2}\beta x^2}.$$

Integrals of the form

$$I_n(\beta) \equiv \int_{-\infty}^{\infty} dx x^{2n} e^{-\beta x^2} = \left(-\frac{d}{d\beta}\right)^n I_0(\beta)$$

occur throughout the problem.

- (a) Show

$$\frac{I_n(\beta)}{I_0(\beta)} = \frac{(2n-1)!!}{(2\beta)^n}$$

where  $(2N+1)!! = (2N+1) \cdot (2N-1) \cdot (2N-3) \dots 3 \cdot 1$

- (b) Show

$$\langle \psi_\beta | H_0 | \psi_\beta \rangle = \frac{1}{4} \left( \beta + \frac{1}{\beta} \right)$$

and check that this gives the correct ground state energy and wavefunction for the unperturbed oscillator.

- (c) Compute  $\langle \psi_\beta | H | \psi_\beta \rangle$  find the condition on  $\beta$  that minimizes the ground state energy. Call the solution to this condition  $\beta(n, \lambda)$ . Show that your upper limit can be written

$$E_0(n, \lambda) = \frac{1}{4} \left( \beta + \frac{1}{\beta} + \frac{1}{n} \left( \beta - \frac{1}{\beta} \right) \right)$$

where  $\beta = \beta(n, \lambda)$ .

- (d) For  $n=1, 2$  and  $3$ , and for  $\lambda=1$ , find  $\beta(n, 1)$  and compute  $E_0(n, 1)$  numerically and compare with the results of first order perturbation theory.

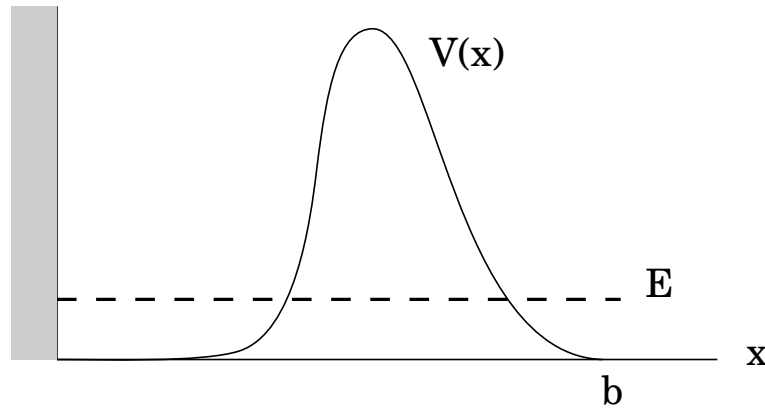


Figure 1: A high potential and a low energy state.

### 3. Phases

*Phase shifts, which determine scattering cross sections, can be estimated in the WKB approximation.*

Consider a particle moving on the half-line  $x \geq 0$  in the presence of a potential like the one shown in Figure 1.

Suppose the potential barrier is very “high” compared to the energy. Then, qualitatively, there are two types of solutions, those that live primarily inside the potential and those that live outside.

A little terminology: for “generic” choices of the energy (always low compared to the barrier height) the particle lives outside the barrier and has a small amplitude to tunnel in. For “special” choices of the energy, the particle lives inside the barrier and has a small amplitude to tunnel out. Whatever the energy, we can parameterize the solution to the Schrödinger equation by a “phase shift” at large  $x$ :

$$\psi(x) \propto \sin(kx + \delta(k)), \text{ for } x \gg b$$

where  $b$  is the “range” of the interaction and  $k = \sqrt{2mE/\hbar^2}$ .  $\delta(k)$  is the shift in the phase of the wave function compared to the case  $V(x) = 0$ , where  $\psi_0(x) \propto \sin kx$ .

- (a) Use the WKB approximation to find the *special* values of the energy.
- (b) For *generic* values of the energy, use the WKB approximation to find an expression for  $\delta(k)$  as an integral over the potential. Is  $\delta(k)$  uniquely determined?
- (c) For the *special* values of the energy you found in part (a), can you say anything about  $\delta(k)$  on the basis of the WKB approximation? Justify your answer.

#### 4. WKB Sum Rules

“Sum Rules”, sums over the properties of energy levels or transition amplitudes, can often be related to fundamental properties of interactions.

Consider a deep, smooth, uniformly attractive potential,  $V(x)$ . Let  $U(x) = -V(x) > 0$ . Suppose  $V(x)$  has very many bound states with binding energies  $B_j$ ,  $j = 1, 2, \dots, N$ . (Of course  $B_j > 0$ .)

The Bohr-Sommerfeld quantization condition reads:

$$\int_{x_1(\kappa)}^{x_2(\kappa)} dx p(\kappa, x) = (n + \frac{1}{2})\pi\hbar \quad (1)$$

where  $p(\kappa, x) = \sqrt{2mU(x) - \hbar^2\kappa^2}$ , and  $x_1(\kappa)$  and  $x_2(\kappa)$  are the classical turning points where  $p(\kappa, x) = 0$ . Note that  $\kappa^2 (= -k^2)$  is directly proportional to the binding energy,  $B = \frac{\hbar^2\kappa^2}{2m}$ . Eq. (1) is, of course, a semi-classical result that we derived in Lecture from the WKB approximation.

(a) Use eq. (1) to derive a “Sum Rule” for the total number of bound states in  $U(x)$ ,

$$N \approx \frac{1}{\pi\hbar} \int_{-\infty}^{\infty} dx \sqrt{2mU(x)}$$

[Hint: What value of  $\kappa$  corresponds to  $n = N$ ?]

Differentiating eq. (1) with respect to  $\kappa$ , we obtain an expression for the density of states (per unit  $\kappa$ ) in the WKB approximation:

$$\rho(\kappa) \equiv \frac{dn}{d\kappa} = \frac{1}{\pi\hbar} \int_{x_1(\kappa)}^{x_2(\kappa)} dx \frac{\partial p}{\partial \kappa} \quad (2)$$

[This is related to the famous estimate from the “old quantum theory”,  $dn = dx dp / 2\pi\hbar$ .]

(b) Use WKB to derive another “Sum Rule”, this time for the sum of the binding energies of all the bound states in  $U(x)$ ,

$$\sum_{j=1}^N B_j = \int d\kappa \rho(\kappa) \left( \frac{\hbar^2\kappa^2}{2m} \right) \approx \frac{2}{3\pi} \sqrt{\frac{2m}{\hbar^2}} \int_{-\infty}^{\infty} dx [U(x)]^{\frac{3}{2}}$$

(c) Can you generalize this result to obtain a sum rule for powers of the binding energy, *i.e.* for  $\sum_{j=1}^N B_j^\ell$  for  $\ell = 0, 1, 2, \dots$ ?

(d) For convenience, set  $\hbar = 2m = 1$ . Evaluate the sum rules of parts (a) and (b) (and part (c) if you are ambitious) for the Pöschl-Teller potential

$$U_{PT}(x) = A \operatorname{sech}^2 x$$

(the integrals can be performed analytically).

When the constant  $A$  is equal to  $p(p+1)$  for  $p = \text{integer}$ , the Schrödinger equation with the Pöschl-Teller potential can be solved exactly in terms of elementary functions. There are  $p$  bound states with binding energies

$$B_j = -j^2, \text{ for } j = 1, 2, \dots, p$$

This enables you to check the accuracy of the WKB sum rules for these values of  $A$ . [You can display your results either as a table or a set of graphs. For example you could plot the WKB estimate for  $\ell = 0, 1, \dots$  versus  $p$  and compare with the exact result for  $p = 1, 2, \dots$ ]

### 5. Transmission and reflection from a Gaussian barrier

Suppose a particle of mass  $m$  is incident on the left from a Gaussian barrier,  $V(x) = V_0 e^{-\frac{1}{2}x^2/a^2}$ , in one dimension. Assume  $V_0 > 0$ . The barrier is high and broad. To be specific, you should assume that  $\Delta \equiv \sqrt{2mV_0}a/\hbar \gg 1$ .

Use the WKB approximation to estimate

- (a) The transmission probability for  $E \ll V_0$ .
- (b) The phase of the transmitted wave when  $E \gg V_0$ .
- (c) The reflection probability when  $E \gg V_0$ .
- (d) For  $\Delta = 10$ , plot the logarithm of the probabilities computed in parts (a) and (c) as functions of  $z = E/V_0$ . Be careful to mark the regions where WKB does not apply.