Quantum Physics III (8.06) — Spring 2016

Assignment 3

Readings

- Griffiths Chapter 9 on time-dependent perturbation theory
- Shankar Chapter 18
- Cohen-Tannoudji, Chapter XIII.

Problem Set 3

1. Semi-classical approximation of the potential $V(x) = \alpha x^4$ (15 points) Consider the Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \alpha x^4\psi = E\psi.$$

Let the energies be $E_0 < E_1 < \ldots$ and define the dimensionless energies $e_n = \frac{E_n}{\gamma}$ where

$$\gamma \equiv \left(\frac{\hbar^4 \alpha}{m^2}\right)^{1/3}$$

In an 8.05 problem set we explored numerical solutions of this potential and found that the first few energies were

$$e_0 = 0.667986$$

$$e_1 = 2.39364$$

$$e_2 = 4.69680$$

$$e_3 = 7.33573$$

$$e_4 = 10.2443$$

$$e_5 = 13.3793$$

In this problem we will show how to estimate these energies using semiclassical methods.

- (a) Assume that the turning points are at $-x_0, x_0$ with $x_0 > 0$. Express the energy E in terms of α and x_0 .
- (b) Use the connection formulae to show (assuming the WKB approximation is valid) that

$$\frac{1}{\hbar} \int_{-x_0}^{x_0} \sqrt{2m(E_n - V(x))} dx = \left(n + \frac{1}{2}\right)\pi$$
(1)

for $n = 0, 1, 2, \dots$

(c) In what follows, we will use \tilde{E}_n to denote the estimate of the n^{th} energy that is obtained from (1) while E_n represents the true energy. Compute the integral in (1) to obtain a formula for $\tilde{e}_n \equiv \tilde{E}_n/\gamma$ in terms of n. The answer should be of the form $\tilde{e}_n = \beta(n+\delta)^{\epsilon}$ for β, δ, ϵ constants to be determined. You may find the following expression useful:

$$\int_0^1 \sqrt{1 - t^4} dt = \frac{\sqrt{\pi} \Gamma(\frac{1}{4})}{8\Gamma(\frac{7}{4})} \approx 0.874019.$$

Write down $\tilde{e}_0, \tilde{e}_1, \tilde{e}_2, \tilde{e}_3, \tilde{e}_4, \tilde{e}_5$ and the relative errors $\left|\frac{\tilde{e}_0 - e_0}{e_0}\right|, \left|\frac{\tilde{e}_2 - e_2}{e_2}\right|$ and $\left|\frac{\tilde{e}_5 - e_5}{e_5}\right|$.

2. Tunneling and the Stark Effect (20 points)

The Stark effect concerns the physics of an atom in an electric field. In this problem, you will explore the possibility that in an electric field, the electron in an atom can tunnel out of the atom, making the atomic bound states unstable. We consider this effect in a simpler one-dimensional analog problem.

Suppose an electron is trapped in a one-dimensional square well of depth V_0 and width d:

$$V(x) = -V_0 \text{ for } |x| < d/2$$

= 0 for $|x| \ge d/2$.

Suppose a weak constant electric field in the x-direction with strength \mathcal{E} is turned on. That is $V \to (V - e\mathcal{E}x)$. Assume throughout this problem that $e\mathcal{E}d \ll \hbar^2/2md^2 \ll V_0$.

- (a) Set $\mathcal{E} = 0$ in this part of the problem. Estimate the ground state energy (i.e. the amount by which the ground state energy is above the bottom of the potential well) by pretending that the well is infinitely deep. (Because $\hbar^2/2md^2 \ll V_0$, this is a good approximation.) Use this estimate of the ground state energy in subsequent parts of the problem. Note that the true ground state energy is lower than what you've estimated, why?
- (b) Sketch the potential with $\mathcal{E} \neq 0$ and explain why the ground state of the $\mathcal{E} = 0$ potential is no longer stable when $\mathcal{E} \neq 0$.
- (c) Use the semiclassical approximation to calculate the barrier penetration factor for the ground state. [You should use the fact that $e\mathcal{E}d \ll \hbar^2/2md^2$ to simplify this part of the problem.]
- (d) Use classical arguments to convert the barrier penetration factor into an estimate of the lifetime of the bound state.
- (e) Now, let's put in numbers that are characteristic of an atomic system. Calculate the lifetime for $V_0 = 20 \text{ eV}$, $d = 2 \times 10^{-8} \text{ cm}$ and an electric field of $7 \times 10^4 \text{ V/cm}$. Compare the lifetime you estimate to the age of the universe.
- (f) Show that the lifetime goes like $\exp(1/\mathcal{E})$, and explain why this result means that this "instability" could not be obtained in any finite order of perturbation theory, treating \mathcal{E} as a perturbation to the Hamiltonian.

3. Tunneling from perturbation theory (20 points) A key feature of tunneling is that the rate is suppressed exponentially by an amount that scales with the barrier width and the square root of the barrier height. By contrast, in second-order perturbation theory the contribution to the energy goes down only like $1/(E_n^0 - E_m^0)$, which we can think of as a barrier height. Nevertheless we will see in this problem how exponential suppression can arise from higher-order perturbation theory.

In this problem we consider a particle localized on a line with a potential 0 at the endpoints and a potential barrier in the middle of height V_0 and width W. Thus the WKB tunneling amplitude is $\exp(-W\sqrt{2mV_0}/\hbar)$.

(a) First suppose the positon of the particle is restricted to sites $0, 1, \ldots, N$. The Hamiltonian consists of two terms. There is a "barrier" term H_0 which is a potential of height V_0 on all sites except 0 and N; i.e.

$$H_0 = V_0 \sum_{x=1}^{N-1} |x\rangle \langle x|, \qquad (2)$$

and a "hopping" term

$$\delta H = -\lambda \sum_{x=1}^{N} |x - 1\rangle \langle x| + |x\rangle \langle x - 1|.$$
(3)

Assume that $\lambda \ll V_0$.



Figure 1: A particle is constrained to occupy one of N + 1 nodes (here N = 5) with a barrier potential H_0 from (2) and a hopping term δH from (3).

If there were no hopping term, there would be a two-dimensional ground space spanned by

$$|g_{+}\rangle = \frac{|0\rangle + |N\rangle}{\sqrt{2}}$$
 and $|g_{-}\rangle = \frac{|0\rangle - |N\rangle}{\sqrt{2}}$

(We could also use $|0\rangle$, $|N\rangle$ but will find $|g_{\pm}\rangle$ more convenient.) The hopping term will create a very small splitting between $E_{g_{\pm}} = \langle g_{\pm}|H_0 + \delta H|g_{\pm}\rangle$. To evaluate this we will need to go to higher-order perturbation theory. The formula for the k^{th} -order correction to the energy of the n^{th} eigenstate is

$$E_n^k = \sum_{m_1} \cdots \sum_{m_{k-1}} \frac{\delta H_{n,m_{k-1}} \cdots \delta H_{m_2,m_1} \delta H_{m_1,n}}{(E_n^0 - E_{m_1}^0) \cdots (E_n^0 - E_{m_{k-1}}^0)} + \text{other terms.}$$
(4)

Here m_1, \ldots, m_{k-1} range over all states not in the same degenerate subspace as n and we have used the fact that in the $\{|g_+\rangle, |g_-\rangle, |1\rangle, \ldots, |N-1\rangle\}$ basis, δH has no off-diagonal terms coupling degenerate states.

What is the smallest value of k for which $E_{g_{-}}^{k} - E_{g_{+}}^{k}$ is nonzero? It turns out that the other terms not shown begin to contribute only for higher values of k, and so for the purposes of this problem it is ok to ignore them.

Evaluate the energy splitting for this value of k. Your answer should decrease exponentially with N, since N is analogous to W, but the scaling with V_0 will not look like the WKB case.

(b) Now suppose that the discrete approximation above came from a 1-D Hamiltonian in which we discretized space and replaced the $p^2/2m$ with a finite difference operator. If the lattice spacing is ℓ then the finite-difference operator corresponding to $\frac{d^2}{dx^2}$ is

$$D_{\ell}^2 = \frac{1}{\ell^2} \sum_{x} -2|x\rangle \langle x| + |x\rangle \langle x+1| + |x\rangle \langle x-1|.$$

If we ignore the diagonal part, then the kinetic energy term $\frac{p^2}{2m}$ is thus equivalent to δH from (3). What is the corresponding value of λ ? Suppose that the potential term is a square barrier of width W and take $\ell = W/N$ so this corresponds to N lattice sites.

We see that as we reduce ℓ the energy splitting in (a) goes down since $N = W/\ell$ increases as $\ell \to 0$. This is an artifact of our approximation scheme since the physics of the system should not depend on ℓ . But we cannot make ℓ arbitrarily small if we want the perturbation-theory argument to work. How should ℓ scale with V_0 and the other parameters so that $\lambda \ll V_0$? More concretely let us set λ/V_0 equal to a dimensionless constant $\epsilon \ll 1$ which we can keep fixed by adjusting ℓ . Estimate the energy splitting as a function of ϵ , W, V_0 , m and \hbar .

(c) Part (a) and (b) have given estimates of the splitting in energies of $|g_{\pm}\rangle$ but have not directly addressed tunneling. In this part, suppose that the Hamiltonian is simply

$$H = E_+ |g_+\rangle \langle g_+| + E_- |g_-\rangle \langle g_-|$$

and define $\Delta = E_- - E_+$. Suppose that we begin at time 0 in the state $|0\rangle$, and after time t we measure whether the particle is in state $|0\rangle$ or $|N\rangle$. At what time t will we find the state in position N with probability 1? Using the energy splitting from (b) above, what can you say about how the tunneling rate scales with W and V_0 ? How does your answer compare with the WKB prediction?

4. A Time-Dependent Two-State System (15 points)

Consider a two-state system with Hamiltonian

$$H(t) = \left(\begin{array}{cc} +E & v(t) \\ v(t) & -E \end{array}\right)$$

where v(t) is real and $\int_{-\infty}^{\infty} |v(t)|$ is finite. We will label the states as

$$|1\rangle = \begin{pmatrix} 1\\ 0 \end{pmatrix}, \qquad |2\rangle = \begin{pmatrix} 0\\ 1 \end{pmatrix}. \tag{5}$$

- (a) Suppose that at $t = -\infty$ the system is in the state $|2\rangle$. Use time-dependent perturbation theory to determine the probability that at $t = +\infty$ the system is in the state $|1\rangle$, to lowest order in v.
- (b) If E = 0, the eigenstates of H(t) can be chosen to be independent of t. Use this fact to calculate the probability of a transition from $|2\rangle$ to $|1\rangle$ exactly, in this case. What is the result obtained from time-dependent perturbation theory in this case? What is the condition that the perturbative result is a good approximation to the exact result?

In both parts, your answers can be left in terms of integrals involving v(t).

5. Atom and photon (20 points) Model an atom as a two-level system with ground state $|g\rangle$ and excited state $|e\rangle$ and energy splitting $\hbar\omega_a$. Suppose it interacts with an electromagnetic field of frequency ω_p , which we model as a harmonic oscillator. Without interactions the Hamiltonian would be

$$H_{0} = \frac{\hbar\omega_{a}}{2} \left(|e\rangle\langle e| - |g\rangle\langle g| \right) \otimes I + \hbar\omega_{p} I \otimes \left(\hat{a}^{\dagger}\hat{a} + \frac{1}{2} \right)$$
$$= \frac{\hbar\omega_{a}}{2} \sigma_{z} \otimes I + \hbar\omega_{p} I \otimes \left(\hat{a}^{\dagger}\hat{a} + \frac{1}{2} \right)$$

Since the electric field strength is proportional to $\hat{a} + \hat{a}^{\dagger}$, we can model an atom-photon interaction by

$$\delta H = \alpha \left(|g\rangle \langle e| + |e\rangle \langle g| \right) \otimes \left(\hat{a} + \hat{a}^{\dagger} \right)$$

for some constant α .

- (a) In the rotating frame, we have $\delta H(t) = e^{iH_0t/\hbar} \delta H e^{-iH_0t/\hbar}$. Compute $\delta H(t)$.
- (b) Set $\omega_a = \omega_p \equiv \omega$. Compute $\int_0^t dt' \delta H(t')$. If $t \gg 1/\omega$, then which terms can we neglect? [Hint: You should be left with one term that can be interpreted as absorption and another that can be interpreted as spontaneous/stimulated emission.]
- 6. Gaussian pulse (10 points) Let H_0 be a Hamiltonian with spectrum and energies given by $H_0|n\rangle = E_n|n\rangle$ for n = 0, 1, 2, ... Suppose we apply a perturbation

$$\delta H(t) = \frac{\exp\left(-\frac{t^2}{2\tau^2}\right)}{\sqrt{2\pi\tau^2}} \hat{V}$$

where \hat{V} is an arbitrary time-independent Hermitian operator and $\tau > 0$ is a constant with units of time. If our system starts in state $|0\rangle$ at time $-\infty$, using first-order timedependent perturbation theory, what is the probability that our system is in state $|n\rangle$ at time ∞ ? What happens in the limits $\tau \to 0$ and $\tau \to \infty$? You should express your answers in terms of the matrix elements $V_{mn} \equiv \langle m | \hat{V} | n \rangle$.

8.06 Quantum Physics III Spring 2016

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