Quantum Physics III (8.06) Spring 2007
FINAL EXAMINATION
Monday May 21, 9:00 am
You have 3 hours.

There are 10 problems, totalling 180 points. Do all problems.

Answer all problems in the white books provided. Write YOUR NAME on EACH white book you use. Budget your time wisely, using the point values as a guide. Note also that shorter problems may not always be easier problems.

No books, notes or calculators allowed.

Some potentially useful information

- **Schrödinger equation**

$$i\hbar\frac{d}{dt}|\psi(t)\rangle = H(t)|\psi(t)\rangle$$

For an energy eigenstate ψ of energy E

$$\psi(t) = e^{-\frac{i}{\hbar}Et}\psi(0)$$

and the Schrodinger equation reduces to an eigenvalue equation

$$H\psi = E\psi$$

- **Harmonic Oscillator**

$$\hat{H} = \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega^2\hat{x}^2$$

where

$$[\hat{x}, \hat{p}] = i\hbar\ .$$

This Hamiltonian can be rewritten as

$$\hat{H} = \hbar\omega\left(\hat{N} + \frac{1}{2}\right)$$

where $\hat{N} = \hat{a}^\dagger\hat{a}$, and the operators $\hat{a}$ and $\hat{a}^\dagger$ are given by

$$\hat{a} = \frac{1}{\sqrt{2m\omega\hbar}}\left(m\omega\hat{x} + i\hat{p}\right)\ ,\qquad \hat{a}^\dagger = \frac{1}{\sqrt{2m\omega\hbar}}\left(m\omega\hat{x} - i\hat{p}\right)\ ,$$

and satisfy

$$[\hat{a}, \hat{a}^\dagger] = 1\ .$$

Conversely

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a} + \hat{a}^\dagger),\qquad \hat{p} = \frac{1}{i}\sqrt{\frac{\hbar m\omega}{2}}(\hat{a} - \hat{a}^\dagger)$$

The action of $\hat{a}$ and $\hat{a}^\dagger$ on eigenstates of $\hat{N}$ is given by

$$\hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle\ ,\quad \hat{a}|n\rangle = \sqrt{n}|n-1\rangle\ .$$

The ground state wave function is

$$\langle x|0\rangle = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{m\omega}{2\hbar}x^2\right)\ .$$

- **Natural units**

  In the natural units, the dimension of any physical quantity can be written as

$$E^a \hbar^b c^d$$

  where E denotes energy whose unit is normally taken to be eV. Some examples

$$[m] = E/c^2$$

$$[L] = \hbar c\, E^{-1}$$

$$[t] = \hbar E^{-1}$$

- **Particle in an Electric and/or Magnetic Field:**

  The Hamiltonian for a particle with charge q in a magnetic field and electric field

$$\vec{B} = \vec{\nabla} \times \vec{A}, \qquad \vec{E} = -\vec{\nabla}\phi - \frac{1}{c}\frac{\partial \vec{A}}{\partial t}$$

  is:

$$H = \frac{1}{2m}\left(\vec{p} - \frac{q}{c}\vec{A}\right)^2 + q\phi \tag{1}$$

  Gauge invariance:

  If $\psi(\vec{x}, t)$ solves the Schrödinger equation defined by the Hamiltonian (1), then

$$\psi'(\vec{x}, t) = \exp\left(-\frac{iq}{\hbar c} f(\vec{x}, t)\right)\psi(\vec{x}, t)$$

  solves the Schrödinger equation obtained upon replacing $\vec{A}$ by $\vec{A}' = \vec{A} - \vec{\nabla} f$ and replacing ϕ by $\phi' = \phi + (1/c)\partial f/\partial t$.

- **Electron in a magnetic field: spin Hamiltonian**

  The Hamiltonian for the spin is given by

$$H = \frac{e}{m}\vec{S} \cdot \vec{B} = \mu_B \vec{\sigma} \cdot \vec{B}$$

  where

$$\vec{S} = \frac{\hbar}{2}\vec{\sigma}, \qquad \mu_B = \frac{e\hbar}{2m}$$

  and

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \;;\; \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \;;\; \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

- **Time independent perturbation theory:**

  Suppose that

$$H = H_0 + H'$$

  where we already know the eigenvalues E_n^0 and eigenstates $|\psi_n^0\rangle$ of H^0:

$$H_0|\psi_n^{(0)}\rangle = E_n^{(0)}|\psi_n^{(0)}\rangle \ .$$

  Then, the eigenvalues and eigenstates of the full Hamiltonian H are:

$$E_n = E_n^{(0)} + H'_{nn} + \sum_{m\neq n} \frac{|H'_{nm}|^2}{E_n^{(0)} - E_m^{(0)}} + \ldots \tag{2}$$

$$|\psi_n\rangle = |\psi_n^{(0)}\rangle + \sum_{m\neq n} \frac{H'_{mn}}{E_n^{(0)} - E_m^{(0)}}|\psi_m^{(0)}\rangle + \ldots \tag{3}$$

  where $H'_{nm} \equiv \langle\psi_n^{(0)}|H'|\psi_m^{(0)}\rangle$.

  If H_0 has degeneracy at $E_n^{(0)}$, first diagonalize H' in the corresponding degenerate subspace, then use equations (2) and (3). In particular $|\psi_n^{(0)}\rangle$ ("good states") should be one of the eigenvectors of H' in the degenerate subspace.

- **Connection Formulae for WKB Wave Functions:**

  At a turning point at $x = a$ at which the classically forbidden region is at $x > a$:

$$\frac{2}{\sqrt{p(x)}}\cos\left[\frac{1}{\hbar}\int_x^a p(x')dx' - \frac{\pi}{4}\right] \quad \leftarrow \quad \frac{1}{\sqrt{\kappa(x)}}\exp\left[-\frac{1}{\hbar}\int_a^x \kappa(x')dx'\right]$$
$$\frac{1}{\sqrt{p(x)}}\cos\left[\frac{1}{\hbar}\int_x^a p(x')dx' + \frac{\pi}{4}\right] \quad \rightarrow \quad \frac{1}{\sqrt{\kappa(x)}}\exp\left[+\frac{1}{\hbar}\int_a^x \kappa(x')dx'\right]$$

  At a turning point at $x = b$ at which the classically forbidden region is at $x < b$:

$$\frac{1}{\sqrt{\kappa(x)}}\exp\left[-\frac{1}{\hbar}\int_x^b \kappa(x')dx'\right] \quad \rightarrow \quad \frac{2}{\sqrt{p(x)}}\cos\left[\frac{1}{\hbar}\int_b^x p(x')dx' - \frac{\pi}{4}\right]$$
$$\frac{1}{\sqrt{\kappa(x)}}\exp\left[+\frac{1}{\hbar}\int_x^b \kappa(x')dx'\right] \quad \leftarrow \quad \frac{1}{\sqrt{p(x)}}\cos\left[\frac{1}{\hbar}\int_b^x p(x')dx' + \frac{\pi}{4}\right]$$

- **Bohr-Sommerfeld quantization condition**

$$\int_a^b dx\, p(x)dx = (n - \frac{1}{2})\pi\hbar, \qquad n = 1, 2, \cdots \tag{4}$$

where a, b are classical turning points. If the potential has a sharp wall on one side, equation (4) becomes

$$\int_a^b dx\, p(x) = (n - \frac{1}{4})\pi\hbar, \qquad n = 1, 2, \cdots \tag{5}$$

If the potential has sharp walls on both side, equation (4) becomes

$$\int_a^b dx\, p(x) = n\pi\hbar, \qquad n = 1, 2, \cdots \tag{6}$$

- **Barrier tunnelling**

$$P \sim e^{-\frac{2}{\hbar}\int_a^b dx\, \kappa(x)}$$

with

$$\kappa(x) = \sqrt{2m(V(x) - E)}$$

and a, b are classical turning points.

- **Adiabatic evolution**

Under adiabatic change of parameters $\vec{R}$ of a Hamiltonian $H(\vec{R})$, if the system is initially in the n-th energy eigenstate, it stays in the same energy eigenstate as the parameters change and acquires a phase factor

$$\psi(t) = e^{-i\theta_n(t) + i\gamma_n(t)} |\psi_n(\vec{R}(t))\rangle$$

with

$$\theta_n = \frac{1}{\hbar}\int_0^t dt'\; E_n(\vec{R}(t'))$$

and

$$\gamma_n(t) = i\int_0^t dt'\; \langle\psi_n(\vec{R}(t'))|\partial_{t'}\psi_n(\vec{R}(t'))\rangle\ .$$

The geometric phase for a spin-$\frac{1}{2}$ particle in a magnetic field: for the spin up state

$$\gamma_+ = -\frac{1}{2}\Omega_C$$

where Ω_C is the solid angle subtended at the origin by the closed curve C traced by the rotating magnetic field .

- **Time Dependent Perturbation Theory**

Consider a system with the Hamiltonian

$$H(t) = H_0 + H'(t)\ .$$

Denote the matrix element of H' between eigenstates of H_0 named $|a\rangle$ and $|b\rangle$ by H'_{ab}. If the system is initially in state $|a\rangle$ at $t = t_0$, the probability that it is in the state $|b\rangle$ at time t is:

$$P_{a\to b} = |c_b(t)|^2$$

with

$$c_b(t) = \frac{1}{i\hbar}\int_{t_0}^{t} dt'\ H'_{ba}(t')e^{i\omega_{ba}t'}, \qquad \omega_{ba} = \frac{E_b - E_a}{\hbar}$$

If H' is periodic in time, i.e.

$$H' = V(\vec{r})\cos\omega t$$

then the *transition rate* from $a \to b$ in the $t \to \infty$ limit is

$$R_{a\to b} = \frac{\pi}{2\hbar^2}|V_{ab}|^2\delta(\omega - \omega_{ab})$$

- **Scattering**:
  - In three dimensions, the wave function $\psi(\vec{r})$ of a particle scattering off a potential $V(\vec{r})$ satisfies the asymptotic boundary condition

    $$\psi(\vec{r}) \to e^{ikz} + \frac{e^{ikr}}{r}f(\theta,\phi), \qquad r \to \infty \tag{7}$$

    (r,θ,ϕ) are spherical coordinates with the scattering center located at $r = 0$ and θ the angle between $\vec{r}$ and z-axis.
  - Born Approximation to Scattering Amplitude

    $$f(\theta,\phi) = f(\vec{q}) = -\frac{m}{2\pi\hbar^2}\int d^3r\,\exp(-i\vec{q}\cdot\vec{r})V(\vec{r})$$

    where $\vec{q} = \vec{k}' - \vec{k}$ is the momentum transfer. If $V(\vec{r})$ is central, then

    $$f(\theta) = -\frac{2m}{\hbar^2 q}\int_0^\infty dr\, rV(r)\sin qr$$

    with

    $$q = 2k\sin\frac{\theta}{2}$$
  - Partial wave expansion: for spherically symmetric potential $V(r)$, the scattering amplitude can be written as

    $$f(\theta) = \sum_{l=0}^{\infty}(2l+1)f_l P_l(\cos\theta)$$

where f_l can be expressed in term the phase shift of the effective one-dimensional problem as

$$f_l = \frac{e^{2i\delta_l} - 1}{2ik} = \frac{e^{i\delta_l}}{k} \sin \delta_l$$

The total cross section is

$$\sigma_{tot} = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \sin^2 \delta_l$$

- **Spherical coordinates in three dimension**

$$x = r \sin\theta \cos\phi; \qquad y = r \sin\theta \sin\phi; \qquad z = r\cos\theta$$

- **Legendre Polynomials**

$$P_0(z) = 1, \qquad P_1(z) = z, \qquad P_2(z) = \frac{3z^2 - 1}{2}, \qquad P_3(z) = \frac{5z^3 - z}{2} \tag{8}$$

- **Useful integrals**

$$\int_{-\infty}^{+\infty} dx \exp\left(-ax^2\right) = \sqrt{\frac{\pi}{a}}$$

$$\int_{-\infty}^{+\infty} dx\, x^2 \exp\left(-ax^2\right) = \frac{1}{2}\sqrt{\frac{\pi}{a^3}}$$

$$\int dx\, x^{\frac{1}{2}} = \frac{2}{3} x^{\frac{3}{2}}$$

1. **Short answer questions (20 points):**

   (a) (2 points) In using the Born-Oppenheimer approximation to study a molecule system, we solve the dynamics of electrons first assuming all nuclei are fixed.

   (b) (2 points) In the Born-Oppenheimer approximation, electrons play no role in the dynamics of the nuclei.

   (c) (2 points) All excited states of the hydrogen atom have zero electric dipole moment.

   (d) (2 points) Partial wave expansion is normally used for high energy scatterings.

   (e) (2 points) A charged particle in an electric and magnetic filed has an expectation value of p that is the same in any gauge.

   (f) (2 points) Aharonov-Bohm effect demonstrates that gauge invariance can not be true in quantum mechanics since the wave function of an electron is affected by the vector potential even in the absence of a magnetic field.

   (g) (2 points) The induced magnetic moment due to the orbital motion of an electron in a magnetic field is in the same direction as the applied field.

   (h) (2 points) In an external magnetic field, to minimize energy, the direction of the spin magnetic moment of an electron is opposite to that of the applied field.

   (i) (2 points) The main physical mechanism underlying Laser is spontaneous emission of light by an excited atom.

   (j) (2 points) The variational method cannot be used to calculate excited states of a system.

2. **Hydrogen spectrum (16 points)**

Consider $n = 2$ states of a hydrogen atom. Electron spin should be considered in this problem. (You can ignore Lamb shift below.)

(a) (2 points) Including fine structure, what is CSCO?

(b) (6 points) List the $n = 2$ eigenstates of the Hamiltonian, including fine structure. Specify which states are degenerate.

(c) (2 points) Now turn on a very strong magnetic field along z direction. Ignore the fine structure, and assume that the magnetic field dependent term in the Hamiltonian is proportional to $\vec{B} \cdot (\vec{L} + 2\vec{S})$. What is CSCO?

(d) (6 points) List all $n = 2$ states and specify the degeneracies.

3. **Electron in a one-dimensional box (20 points)**

Consider a spin-$\frac{1}{2}$ particle (e.g. electron) confined in a one-dimensional infinite square well along x-direction (no motion in y and z directions),

$$\begin{aligned} V &= 0, \qquad 0 < x < 2a \\ &= \infty, \qquad \text{otherwise} \end{aligned} \tag{9}$$

(a) (5 points) Write down the energy eigenfunctions and eigenvalues for the system. What are the degeneracies?

(b) (5 points) Find the lowest order relativistic correction to the ground state energy. When do relativistic corrections become important?

Note that the lowest order relativistic correction gives rise to the following additional term in the Hamiltonian:

$$H' = -\frac{p^4}{8m^3c^2} \ .$$

(c) (10 points) Apply a magnetic field to the system with

$$\begin{aligned} \vec{B}(x) &= B\,\vec{e}_z, \qquad 0 < x < a \\ &= B\,\vec{e}_x, \qquad a < x < 2a \end{aligned} \tag{10}$$

where B is constant. This generates a new term in the Hamiltonian given by

$$H' = \mu \vec{B}(x) \cdot \vec{\sigma} \tag{11}$$

where μ is a constant and $\vec{\sigma}$ are Pauli matrices. Treating H' as a small perturbation, find the new ground state energy to lowest order in μB. (**In this part, ignore relativistic corrections.**)

4. **Born approximation (12 points)**

Consider a particle of mass m and initial momentum $\vec{k} = k\vec{e}_z$ scattering off the potential

$$V(\vec{r}) = V_0 \left[\delta(\vec{r} - \vec{a}) + \delta(\vec{r} + \vec{a})\right] \tag{12}$$

where

$$\vec{a} = a\vec{e}_x$$

is a constant vector.

(a) (3 points) What is the definition of scattering differential cross section? How is it related to the scattering amplitude $f(\theta, \phi)$?

(b) (6 points) What is the scattering amplitude $f(\theta, \phi)$ in the first Born approximation.

(c) (3 points) Write down the expression for the total cross section in the first Born approximation. (**Do NOT evaluate the integrals.**)

5. **Partial wave expansion (16 points)**

In a scattering experiment of particles of energy $E = \frac{\hbar^2 k^2}{2m}$, one finds that the differential cross section can be written as

$$\frac{d\sigma}{d\Omega} = \frac{1}{k^2}\left(\frac{1}{3} + \cos\theta + \frac{9}{4}\cos^2\theta\right) \tag{13}$$

The number multiplying the second term was wrongly calculated. The correct number should be 1.7.

(a) (2 point) What can you say about symmetry properties of the scattering potential? Why?

(b) (2 points) What partial waves (i.e. waves with what values of orbital angular momentum quantum number l) are scattering?

(c) (8 points) What are the corresponding phase shifts for partial waves in (b)?

(d) (4 points) What is the total cross section?

6. **A time-dependent two-state system (21 points)**

Consider a two-state system with basis vectors $|1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $|2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$. In this basis the Hamiltonian is

$$H = E \begin{pmatrix} \cos\left(\frac{\pi t}{2T}\right) & \sin\left(\frac{\pi t}{2T}\right) \\ \sin\left(\frac{\pi t}{2T}\right) & -\cos\left(\frac{\pi t}{2T}\right) \end{pmatrix} \tag{14}$$

where E and T are constants. Suppose at $t = 0$ the system is in state $|1\rangle$. Denote the state at time t by $|\psi(t)\rangle$.

(a) (3 points) What condition must T satisfy in order for the time evolution to be well-approximated as adiabatic?

Below assume the criterion of part (a) is satisfied.

(b) (6 points) What is the probability that the system is in state $|1\rangle$ at time $t = T$?

(c) (3 points) What is the probability that the system is in state $|1\rangle$ at time $t = 2T$?

(d) (3 points) Given an example of a physical system which is described by (14).

(e) (6 points) What is $|\psi(4T)\rangle$? Make sure to include the correct overall phase. (Hint: You do NOT need to do extensive calculations for this part. Use part (d).)

7. **Particle production in an expanding and contracting universe (10 points)**

Consider a harmonic oscillator system with time-dependent frequencies

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2(t)x^2 \ . \tag{15}$$

where

$$\omega^2(t) = \omega^2 + \lambda\omega^2 e^{-\frac{t^2}{T^2}} \ . \tag{16}$$

Treat the dimensionless parameter λ as very small.

If at $t = -\infty$, the system is in the ground state of the harmonic oscillator, what is the probability that the system is in n-th state at $t = +\infty$ (to lowest order in λ)? You should give explicit expressions for all $n \geq 1$.

[Note: this problem can be used to model particle production in an expansion and contracting universe.]

8. **A theorem of one-dimensional Schrodinger systems (16 points)**

Consider two one-dimensional bounded quantum systems

$$H_1 = \frac{p^2}{2m} + V_1(x), \qquad H_2 = \frac{p^2}{2m} + V_2(x)$$

Suppose that $V_1(x) > V_2(x)$ for all x. We will denote the energy eigenvalues of two systems by $E_n^{(1)}$ and $E_n^{(2)}$ respectively, with $n = 1, 2, \cdots$.

(a) (8 points) Use the variational method to prove that the ground state energies of two systems satisfy

$$E_1^{(1)} > E_2^{(1)} \ .$$

(b) (8 points) Use Feynman-Hellman theorem to show that $E_n^{(1)} > E_n^{(2)}$ for all n.

Feynman-Hellman theorem: Suppose $H(\lambda)$ depends on some parameter λ and

$$H(\lambda)\psi_n(\lambda) = E_n(\lambda)\psi_n(\lambda),$$

then

$$\frac{\partial E_n(\lambda)}{\partial \lambda} = \langle \psi_n | \frac{\partial H(\lambda)}{\partial \lambda} | \psi_n \rangle$$

9. **The Bouncing Ball (22 points)**

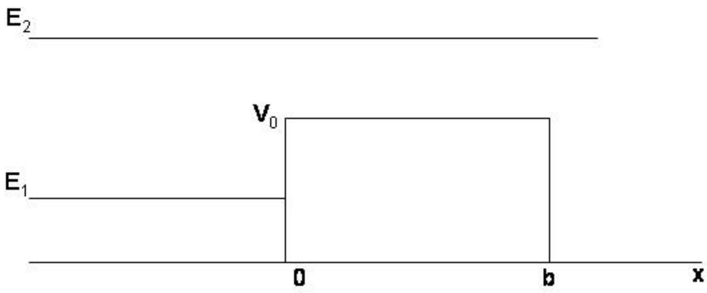
Consider the quantum mechanical analogue to the classical problem of a ball of mass m bouncing elastically on the floor, under the influence of a gravitational potential which can be written as $V(x) = Fx$ (F is a constant). The motion is one-dimensional and is restricted to $x \geq 0$.

(a) (8 points) What is the dimension of F (either cgs or natural units is fine)? Use dimensional analysis to express an energy eigenvalue E in terms of parameters $F, m, \hbar$ up to an overall constant.

(b) (8 points) Find the energy eigenvalues using the WKB approximation. **For convenience of notation: in part (b) and (c) set** $m = \frac{1}{2}$, $F = 1$ **and** $\hbar = 1$**.**

(c) (6 points) Write down a trial wave function with an undetermined parameter. Outline the steps you would use to find a variational estimate of the ground state energy. (You do NOT need to do or simplify the integrals. But write them down explicitly.)

10. **WKB approximation for one-dimensional scattering (27 points)**



Consider a potential barrier of the form indicated in the above figure.

(a) (5 points) Consider an incident plane wave coming from $x = -\infty$ with energy $E_1 = V_0 - K$ $(K > 0)$. The solution to schrodinger equation should satisfy

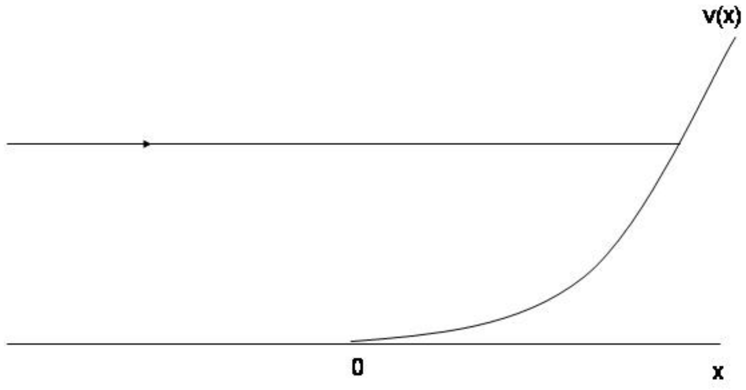
$$\begin{aligned} \psi(x) = &\quad e^{ikx} + re^{-ikx}, \qquad & x < 0 \\ = &\quad te^{ikx}, \qquad & x > b\ . \end{aligned} \tag{17}$$

Use the WKB approximation to estimate $|t|^2$. (**You only need to evaluate the exponential part. You do NOT need to derive the tunnelling formula.**)

(b) (10 points) Consider an incident plane wave coming from $x = -\infty$ with energy $E_2 = V_0 + K$ $(K > 0)$. The solution to schrodinger equation should still have the form (17). Since now $E_2 > V_0$ we expect $r \approx 0$ and $|t| \approx 1$. Thus we can write t as a phase factor

$$t = e^{i\delta}$$

Use the WKB approximation to determine the phase δ.



(c) (12 points) Now consider a one-dimensional potential of the form

$$V(x) = \begin{cases} 0, & x < 0 \\ v(x), & x > 0 \end{cases} \tag{18}$$

where $v(x)$ is some function with the property that $v(x) \to \infty$ as $x \to \infty$ and $v(0) = 0$, as indicated in above figure. In $x < 0$ region the solution to Schrodinger equation can be written as

$$\psi(x) = e^{ikx} + e^{2i\delta} e^{-ikx} \tag{19}$$

with $k = \sqrt{\frac{2mE}{\hbar^2}}$. The first term in (19) is an incident wave and the second term is the reflected wave. Use the WKB approximation to determine δ in (19). [**Hint: You will need to use connection formulas for this part.**]