# Quantum Physics III (8.06) Spring 2006 FINAL EXAMINATION Monday May 22, 1:30 pm You have 3 hours.

There are 11 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  $\psi$  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

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

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

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

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

$$(eV)^a\hbar^bc^d$$

It is often convenient to set  $c = \hbar = 1$ . Then the dimension of any physical quantity can be written in terms of powers of electron Volts. For example

$$[e] = (eV)^0$$
 (dimensionless) 
$$[m] = eV$$
 
$$[L] = eV^{-1}$$
 
$$[t] = eV^{-1}$$

#### • 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  $\phi$  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:

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

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

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

$$\frac{1}{\sqrt{p(x)}}\cos\left[\frac{1}{\hbar}\int_{x}^{a}p(x')dx' + \frac{\pi}{4}\right] \rightarrow \frac{1}{\sqrt{\kappa(x)}}\exp\left[+\frac{1}{\hbar}\int_{a}^{x}\kappa(x')dx'\right]$$

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

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

$$\frac{1}{\sqrt{\kappa(x)}} \exp\left[+\frac{1}{\hbar} \int_{x}^{b} \kappa(x') dx'\right] \leftarrow \frac{1}{\sqrt{p(x)}} \cos\left[\frac{1}{\hbar} \int_{b}^{x} p(x') dx' + \frac{\pi}{4}\right]$$

#### • Bohr-Sommerfeld quantization condition

$$\int_{a}^{b} dx \, p(x)dx = (n - \frac{1}{2})\pi\hbar, \qquad n = 1, 2, \dots$$
 (4)

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

$$\int_{a}^{b} dx \, p(x) = (n - \frac{1}{4})\pi\hbar, \qquad n = 1, 2, \dots$$
 (5)

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

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

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

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

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

where  $\Omega_C$  is the solid angle subtended by C at the origin.

#### • 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

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

 $(r, \theta, \phi)$  are spherical coordinates with the scattering center located at r = 0 and  $\theta$  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

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

with

$$q = 2k\sin\frac{\theta}{2}$$

#### • Polar coordinates in two-dimension

Polar Coordinates

$$x = \rho \cos \theta; \quad y = \rho \sin \theta;$$

$$\nabla^2 f = \frac{1}{\rho} \partial_{\rho} (\rho \partial_{\rho} f) + \frac{1}{\rho^2} \partial_{\theta}^2 f \tag{8}$$

$$= \frac{1}{\sqrt{\rho}}\partial_{\rho}^{2}(\sqrt{\rho}f) + \frac{1}{4\rho^{2}}f + \frac{1}{\rho^{2}}\partial_{\theta}^{2}f \tag{9}$$

• 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. True or False (20 points):

- (a) (2 points) Coulomb interaction between electrons does NOT play a significant role in finding the ground energy of the Helium atom.
- (b) (2 points) Aharonov-Bohm effect is an example of nontrivial Berry's phase.
- (c) (2 points) In MSW mechanism, a muon neutrino created inside the Sun is adiabatically turned into an electron neutrino as it propagates through the Sun.
- (d) (2 points) If you dump some matter onto a stable neutron star, increasing its mass, its radius becomes bigger.
- (e) (2 points) Once you include relativistic and spin-orbit corrections, there are no remaining degeneracies in the hydrogen spectrum (i.e. every energy eigenstate has a different energy eigenvalue).
- (f) (2 points) A charged particle in an electric and magnetic field has an expectation value of x that is the same in any gauge.
- (g) (2 points) A classical computer cannot simulate a quantum computer.
- (h) (2 points) Shor algorithm for factorizing a large integer achieves an exponential speedup compared to the best classical algorithm.
- (i) (2 points) The ground state of a hydrogen atom in a weak magnetic field splits into two levels (ignore hyperfine splitting in this problem).
- (j) (2 points) Laser is based on the stimulated emission of photons.

# 2. Short answer questions (10 points)

- (a) (3 points) In a scattering experiment, how do we measure the scattering differential cross section?
- (b) (2 points) State in words the condition for the validity of the first Born approximation for scattering.
- (c) (5 points) Consider a diatomic molecule ion with a single electron. Let the coordinate separation of the two atoms be given by the three component vector  $\vec{R}$ . Let the coordinates of the electron be described by vector  $\vec{r}$ . Ignore spin. The Hamiltonian (in coordinate space) of the full system can be written as

$$H = -\frac{\hbar^2}{2M_N} \nabla_R^2 - \frac{\hbar^2}{2m_e} \nabla_r^2 + V_N(R) + V_e(r, R)$$
 (10)

The first term is the kinetic energy of the nuclei ( $M_N$  is the reduced mass). The second is the kinetic energy of the electrons. The third is the Coulomb potential energy of the two nuclei and the fourth term is the Coulomb interaction between the electron and the nuclei. Outline in a few sentences your strategy of attacking this problem (If necessary, you can include equations in your answer, but no calculation is required.)

# 3. The Quantum Dipole-Dipole Interaction (10 points)

When a neutral, but polarizable, molecule is placed in an electric field  $\vec{E}$ , it develops an induced electric dipole moment  $\vec{d}$  proportional to  $\vec{E}$ ,

$$\vec{d} = \alpha \vec{E} \ . \tag{11}$$

 $\vec{d}$  has dimensions of charge×length. The constant  $\alpha$  is called the polarizability, and is a property of the molecule in question.

- (a) (2 points) What are the units for force and electric field in natural units? (In your answer, you can set  $\hbar$  and c to 1.)
- (b) (3 points) What are the units of  $\alpha$  defined in (11) in natural units? (In your answer, you can set  $\hbar$  and c to 1.)
- (c) (5 points) Consider the force between two neutral polarizable molecules. Quantum fluctuations in one molecule give rise to an electric field that polarizes the other, and vice versa. This leads to a Casimir force between the two molecules, with strength given by

$$|\vec{F}| = k \frac{\alpha_1 \alpha_2}{R^p}$$

where R is the separation between the molecules, where  $\alpha_1$  and  $\alpha_2$  are the polarizabilities of the two molecules, and where the constant k can only depend on  $\hbar$  and/or c.

Find the power p by dimensional analysis.

# 4. A Particle in a Weak Electric Field (22 points)

A particle of mass m and electric charge q is confined within a one dimensional well, with

$$V(x) = -V_0 |x| < \frac{a}{2}$$
 (12)  
= 0 |x| >  $\frac{a}{2}$ 

$$= 0 |x| > \frac{a}{2} (13)$$

Assume that  $V_0 \gg \frac{\pi^2 \hbar^2}{ma^2}$ , i.e. the wall is deep.

- (a) (5 points) Using the WKB approximation, find the energy quantization condition for a bound state with E < 0.
- (b) (3 points) Estimate the number of bound states of the system.

A weak external electric field  $\mathcal{E}_0$  (in the x-direction) is applied to the system. Choose the zero of electrostatic potential  $\phi$  so that  $\phi(x) = 0$  for x = 0. Assume that  $V_0 \gg e\mathcal{E}_0 a$ .

- (c) (3 points) Now the bound states of the system are no longer stable. Explain why (use a figure if necessary).
- (d) (6 points) Find the barrier penetration factor for the ground state. To leading order, you can assume that the particle sits at x = 0 with an energy  $-V_0$ .
- (e) (5 points) Estimate the life time of the ground state.

# 5. Derivation of band gap from perturbation theory (15 points)

A particle of mass m moves in a one-dimensional box of size L with a periodic potential

 $V(x) = V_0 \cos\left(\frac{2\pi x}{a}\right)$ 

where L = Na, with N a very large even integer (say  $10^{10}$ ). We impose the periodic boundary condition on wave functions, i.e.

$$\psi(x) = \psi(x+L)$$

- (a) (2 points) What does the Bloch theorem say about the wave functions of energy eigenstates?
- (b) (4 points) First consider  $V_0 = 0$ . Consider plane waves which satisfy the condition

$$\phi(x+a) = -\phi(x)$$

What is the energy spectrum for this class of wave functions?

- (c) (8 points) Now consider  $V_0$  small (i.e.  $V_0 \ll \frac{\hbar^2}{ma^2}$ ), calculate the lowest two energy eigenvalues by first order perturbation theory for the class of wave functions considered in (b).
- (d) (1 point) Explain the significance of the results of (c).

# 6. A slow field reversal (20 points)

An electron is held in a spin up state along the z-axis by a magnetic field,  $\vec{B} = B_0 \hat{z}$ . An experimenter would like to reverse the electron spin adiabatically.

- (a) (3 points) Explain why, if he had the choice he would slowly rotate the magnetic field until it pointed in the  $-\hat{z}$  direction, as opposed to slowly reversing the field.
- (b) (3 points) Since it is expensive to rotate a magnet, and cheap to just reverse the current, the experimenter decides it is almost as good just to reverse the field, provided he places the apparatus in a weak permanent magnet with its field  $\vec{B}_1$  pointing some direction in the xy-plane. What is his reasoning?
- (c) (4 points) Now suppose the weak permanent magnetic field described in (b) is along x direction with a magnitude  $B_1 \ll B_0$ . The experimenter slowly reverses the magnetic field along z direction in the following manner  $B_z(t) = -B_0 \frac{t}{T}$  for  $-T \leq t \leq T$ . Write down the Hamiltonian of the system during the reversion process.
- (d) (5 points) How large T has to be for the adiabatic condition to be valid. (derive an inequality that T has to satisfy)
- (e) (5 points) Now set  $B_1 = 0$ . The experimenter slowly rotates the magnetic field originally pointing in z direction along a full circle in the x z plane during a time interval T. In the process he keeps the magnitude  $B_0$  of the magnetic field fixed. Assuming the adiabatic condition is satisfied, what is the total phase change for the electron wave function after the magnetic field returns to its original z-direction? (Hint: the total phase includes both the dynamical phase and Berry's phase.)

# 7. Born approximation (12 points)

Consider a particle of mass m scattering off a delta-shell potential in 3d

$$V(r) = V_0 b \, \delta(r - b)$$

- (a) (5 points) What is the scattering amplitude a particle with energy  $\frac{\hbar^2 k^2}{2m}$  in the first order Born approximation?
- (b) (3 points) What is the differential cross section in the first order Born approximation?
- (c) (4 points) What is the total cross section in the limit  $k \to 0$ ?

# 8. Forced harmonic oscillator (15 points)

Consider an harmonic oscillator perturbed under a time dependent external potential for  $t \ge 0$ 

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 + V(x)f(t)$$

The system is in ground state  $|0\rangle$  at t=0.

(a) (9 points) Suppose

$$V(x) = \lambda x, \qquad f(t) = e^{-\mu t}$$

To lowest order in  $\lambda$  what is the probability that system is in n-th state at  $t = \infty$ ? (You should give explicit expressions for all  $n \ge 1$ .)

(b) (6 points) Now take

$$V(x) = \lambda x^8, \qquad f(t) = \cos \Omega t$$

For what values of  $\Omega$  that the harmonic oscillator has a nonzero probability (to lowest order in  $\lambda$ ) to jump to an excited state? (You only need to write down the answer and give a brief explanation for your answer in words. No intermediate calculation is required.)

# 9. Two variational proofs (20 points)

- (a) (8 points) Prove that, in time-independent perturbation theory, the sum of the second order, third order, fourth order plus all higher order corrections to the ground state energy of a quantum system must be either zero or negative.
- (b) (12 points) Consider a particle of mass m in a one-dimensional potential. The Hamiltonian is  $H = \frac{p^2}{2m} + V(x)$ . The potential has the following properties:

$$V(x) < 0 \qquad |x| < a \tag{14}$$

$$= 0 |x| > a (15)$$

Use the variational principle to prove that there is at least one bound state solution. [Hint: Take e.g. the trial wave function to be a Gaussian  $N(\alpha)e^{-\frac{1}{2}\alpha^2x^2}$  and consider the limit  $\alpha$  small, i.e. the width of the Gaussian becomes large in the limit.]

# 10. Boundary conditions for scattering problems (20 points)

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

$$\psi(\vec{r}) \to e^{ikz} + \frac{e^{ikr}}{r} f(\theta, \phi), \qquad r \to \infty$$
 (16)

The first term in (16) is the incoming plane wave along z-direction and the second term is the scattered spherical wave.  $(r, \theta, \phi)$  are spherical coordinates with the scattering center located at r = 0 and  $\theta$  the angle between  $\vec{r}$  and z-axis.

- (a) (4 points) If the scattering potential  $V(\vec{r})$  is central, i.e.  $V(\vec{r}) = V(r)$ , give argument that f should only depend on  $\theta$ . Should  $f(\theta, \phi)$  be independent of  $\theta$  as well? Why?
- (b) (2 points) Reconsider the question (a) for the limit  $k \to 0$ .
- (c) (4 points) Now let us consider a scattering problem in one dimension  $(-\infty < x < +\infty)$  with the incoming plane wave in the +x direction. What should be the boundary condition we impose on the wave function (i.e. analogue of (16) for 1d scattering)?
- (d) (10 points) Now let us consider a scattering problem in two dimensions with the incoming plane wave in x direction. What should be the boundary condition we impose on the wave function (i.e. analogue of (16) for 2d scattering)?

# 11. The Landau Problem Revisited (16 points)

Consider a particle of mass m and charge q moving in a uniform magnetic field B directed along the z-axis. We will only consider the motion in x-y plane.

- (a) (8 points) Find the energy spectrum of the particle.
- (b) (8 points) Let the wave function of the particle initially (at t=0) have the form

$$\Psi(x, y; 0) = \psi(x, y) \tag{17}$$

Show that the wave function  $\Psi(x,y;t)$  at time t, aside from an arbitrary phase factor, is periodic in t with a period T, where  $T = \frac{2\pi}{\omega_L}$  is the period of the classical motion of the particle in the magnetic field and  $\omega_L$  is the classical cyclotron frequency.