# NIU Physics PhD Candidacy Exam - Fall 2014

# Quantum Mechanics

## Do Only Three Out Of Four Problems

#### I. ELECTRON IN WELL [(12+10+18) PTS]

An electron (ignore the effects of spin) is in a 1-dimensional potential well V(x) with

$$V(x) = \left\{ \begin{array}{ll} 0 \, \mathrm{eV} & \text{for } \ 0 < x < 0.4 \mathrm{nm} \ \text{ and } \ x > 10.4 \mathrm{nm} \\ 200 \, \mathrm{eV} & \text{for } \ x < 0 \ \ \text{ and } \ 0.4 \mathrm{nm} < x < 10.4 \mathrm{nm} \end{array} \right.$$

- a) What are the lowest two energies (in eV) for the bound states in the region with 0 < x < 0.4nm? How do they compare to the energies levels of an infinite well with the same width?
- b) How many bound states are in this well?
- c) If an electron is initially in the well, what is the relative probability for an electron in the lowest energy state to tunnel through the barrier compared to an electron in the second lowest energy state? Give the result in a number good to a factor of 10.

Electron mass =  $0.5 \text{MeV/c}^2$ ;  $\hbar c = 197 \text{ eV nm}$ ;  $\hbar c = 1240 \text{ eV nm}$ 

#### II. SLIGHTLY RELATIVISTIC 1D HARMONIC OSCILLATOR [(6+10+12+12) PTS]

You know that the concept of potential energy is not applicable in relativistic situations. One consequence of this is that the only fully relativistic quantum theories possible are quantum field theories. However, there do exist situations where a particle's motion is "slightly relativistic" (e.g.,  $v/c \sim 0.1$ ) and where the force responds quickly enough to the particle's position that the potential energy concept has approximate validity.

Here we consider the one-dimensional harmonic oscillator, defined by the Hamiltonian

$$\hat{\mathcal{H}}_0 = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{x}^2.$$

Reminder: The eigenvalues of the harmonic oscillator are  $E_n=\hbar\omega\left(n+\frac{1}{2}\right)$  and the eigenstates can be expressed as  $|n\rangle=\frac{1}{\sqrt{n!}}(\hat{a}^{\dagger})^n\,|0\rangle$  with the creation  $(\hat{a}^{\dagger})$ /annihilation  $(\hat{a})$  operators given by  $(\hat{x}/x_0\pm i\hat{p}/p_0)/\sqrt{2}$ , respectively  $[x_0=\sqrt{\hbar/(m\omega)},p_0=\sqrt{m\hbar\omega}]$ .  $\hat{a}^{\dagger}\,|n\rangle=\sqrt{n+1}\,|n+1\rangle$  and  $\hat{a}\,|n\rangle=\sqrt{n}\,|n-1\rangle$ .

- a) Using the relativistic energy relation  $E=(m^2c^4+p^2c^2)^{1/2}$ , derive the  $\hat{p}^4$  order correction to the harmonic oscillator Hamiltonian given above.
- b) Calculate  $\langle n|\,\hat{p}^4\,|0\rangle$ . Hint: The result has the form  $p_0^4\,(C_0\delta_{n,0}+C_2\delta_{n,2}+C_4\delta_{n,4})$ , with numerical prefactors  $C_i$  that you will find.
- c) Calculate the leading non-vanishing energy shift of the ground state due to this relativistic perturbation.
- d) Calculate the leading corrections to the ground state eigenvector  $|0\rangle$ .

#### III. COUPLED SPINS [(18+6+16) PTS]

Consider two spatially localized spins 1/2,  $S_1$  and  $S_2$ , coupled by a transverse exchange interaction and in an inhomogeneous magnetic field. The Hamiltonian is:

$$H = b_1 S_{1z} + b_2 S_{2z} - k(S_1^+ S_2^- + S_1^- S_2^+),$$

where  $b_1$  and  $b_2$  are proportional to the magnetic fields at the two sites and k measures the strength of the exchange coupling, and  $S_1^\pm = S_{1x} \pm i S_{1y}$  and  $S_2^\pm = S_{2x} \pm i S_{2y}$ .

- a) Find the energy eigenvalues.
- b) If both spins are in the +z directions at time t=0, what is the probability that they will both be in the +z direction at a later time t?
- c) If  $b_1 = b_2$ , and at time t = 0 the spin  $S_1$  is in the +z direction and  $S_2$  is in the -z direction, then what is the probability that  $S_1$  will be in the -z direction at a later time t?

#### IV. SPHERICAL POTENTIAL WELL [(10+10+10+10) PTS]

Consider a spherical potential well with

$$U(r) = 0$$
  $r < a$  ;  $U(r) = \infty$   $r > a$ 

- a) Give the radial part of the Hamiltonian for r < a.
- b) We are now only interested in the wavefunction for l=0. Give the general solution of the differential equation by trying a solution R=P/r. (Normalization is not necessary).
- c) Determine the behavior of the wavefunction for  $r \to 0$ . What does the condition that the wavefunction should not diverge at r = 0 imply?
- d) Determine the energy eigenvalues.

# NIU Physics PhD Candidacy Exam - Spring 2014

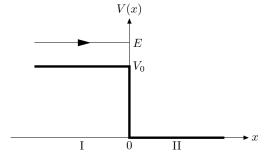
# Quantum Mechanics

## Do Only Three Out Of Four Problems

#### I. POTENTIAL STEP [(10+15+15) PTS]

Let us consider a particle in a potential  $V(x)=V_0\Theta(-x)$ . As shown in the figure, the particle shall come from the left with energy  $E>V_0$  towards the step at x=0.

- a) Make an ansatz for the wave function in regions x < 0 (I) and x > 0 (II) and solve the Schrödinger equation in these regions.
- b) Use the continuity conditions at x=0 and determine the coefficients you used in a) as functions of  $V_0$  and E.
- c) Calculate the probability that the particle is reflected at the potential step.



#### II. BASIS TRANSFORMATION [(10+14+16) PTS]

Let us consider a three-dimensional basis  $|0\rangle$ ,  $|k_0\rangle$ , and  $|-k_0\rangle$  where the basis functions are given by

$$\psi_k(x) = \langle x|k\rangle = \frac{1}{\sqrt{2\pi}}e^{ikx}.$$

a) Write the Hamiltonian

$$\mathbf{H} = -2|0\rangle\langle 0| - \sum_{k,k'=0,\pm k_0;\ k\neq k'} |k\rangle\langle k'|$$

in matrix form.

b) We want to transform the basis from exponential into sines and cosines. We can do this by combining the  $|\pm k_0\rangle$  using the unitary transformation

$$|\psi\rangle = U|\psi'\rangle \quad \text{with} \quad U = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix}.$$

Express the Hamiltonian in the new basis.

c) Calculate the eigenvalues and eigenvectors of the Hamiltonian (Express the result in bra-ket notation).

## III. BOUND STATES [(14+10+16) PTS]

Let the potential V=0 for  $r < a_0$  (the Bohr radius) and  $V=\infty$  for  $r > a_0$ . V is a function of the radius r only.

- a) What is the energy of an electron in the lowest energy state of this potential?
- b) How does that compare to the energy of the 1S state of Hydrogen?
- c) What is the approximate energy of the lowest energy state with angular momentum greater than 0 (you can leave this result in integral form)?

# IV. SPIN PRECESSION [(8+8+8+8) PTS]

We consider a spin-1/2 particle in an external magnetic field  $B_z$ , i.e., the Hamiltonian is  $H=-\mu B_z S_z$  with spin magnetic moment  $\mu$  and  $S_z$  is the z component of the spin operator.

- a) Suppose the particle is initially (time t=0) in an eigenstate  $|+,x\rangle$  of spin  $S_x$  with eigenvalue  $+\hbar/2$ . Express  $|+,x\rangle$  in terms of the eigenstates  $|+,z\rangle$  and  $|-,z\rangle$  of spin  $S_z$ .
- b) Evaluate the time evolution of the state  $|+,x\rangle$  in the Schrödinger picture.
- c) Evaluate the time evolution of the expectation value  $\langle S_x \rangle$  in the Schrödinger picture, assuming that the particle is at time t=0 in the state  $|+,x\rangle$ .
- d) Solve the Heisenberg equation of motion for the operator  $S_x^{\mathrm{H}}(t)$  in the Heisenberg picture.
- e) Show that the time-dependent expectation value  $\left\langle S_x^{\rm H}(t) \right\rangle$  in the Heisenberg picture equals your result from (c) obtained in the Schrödinger picture.

# NIU Physics PhD Candidacy Exam - Fall 2013

# Quantum Mechanics

## Do Only Three Out Of Four Problems

# I. PARTICLE IN POTENTIAL WELL [(16+12+12) PTS]

Here we consider a particle of mass m confined in a one-dimensional potential well defined by

$$U(x) = \begin{cases} \alpha \delta(x), & |x| < a \\ \infty, & |x| \ge a \end{cases}$$

for a>0 and  $\alpha>0$ . The energy levels (eigenvalues)  $E_n$  can be calculated without perturbation theory.

- a) For  $ma\alpha/\hbar^2 \gg 1$ , show that the lowest energy levels  $n \sim 1$  are pairs of close lying levels.
- b) Find the spectrum for large energies  $n \gg 1$ .
- c) Find the energy levels for  $\alpha < 0$ .

#### **II. DENSITY MATRIX** [(10+10+5+15) PTS]

Let us consider a system in a (normalized) pure quantum state  $|\psi\rangle$  and define the operator

$$\hat{\rho} \equiv |\psi\rangle \langle \psi|$$
,

which is called the density matrix.

- a) Show that the expectation value of an observable associated with the operator  $\hat{A}$  in  $|\psi\rangle$  is  $\mathrm{Tr}(\hat{\rho}\hat{A})$ .
- b) Frequently physicists don't know exactly which quantum state their system is in. (For example, silver atoms coming out of an oven are in states of definite  $\mu$  projection, but there is no way to know which state any given atom is in.) In this case there are two different sources of measurement uncertainty: first, we don't know what state they system is in (statistical uncertainty, due to our ignorance) and second, even if we did know, we couldn't predict the result of every measurement (quantum uncertainty, due to the way the world works). The density matrix formalism neatly handles both kinds of uncertainty at once. If the system could be in any of the states  $|\psi_1\rangle$ ,  $|\psi_2\rangle$ , ...,  $|\psi_i\rangle$ , ... (which do not necessarily form a basis set), and if it has probability  $p_i$  of being in state  $|\psi_i\rangle$ , then the density matrix

$$\hat{\rho} = \sum_{i} p_i |\psi_i\rangle \langle \psi_i|$$

is associate with the system. Show that that expectation value of the observable associated with  $\hat{A}$  is still given by  $\mathrm{Tr}(\hat{\rho}\hat{A})$ .

- c) Calculate  $Tr(\hat{\rho})$ .
- d) Now we consider the example of two spin-1/2 particles. Give the density matrix for the following cases in  $\{|+\rangle, |-\rangle\}$ -basis ( $\pm$  refer to the sign of the eigenvalue of the spin operator):
  - Both spins have the same orientation.
  - The total spin is zero.

*Hint:* The trace can be written as  $\operatorname{Tr}(\hat{A}) = \sum_k \langle \phi_k | \hat{A} | \phi_k \rangle$ , where the  $|\phi_k\rangle$  form an orthonormal basis.

#### III. ELECTRON IN A HOMOGENEOUS MAGNETIC FIELD [(16+12+12) PTS]

Let us consider electrons (mass  $\mu$ , charge -e), which move in a spatially homogeneous constant magnetic field in the x-y plane.

a) Show that the Hamiltonian can be written as

$$\hat{\mathcal{H}} = \frac{2}{\mu} \left[ -\hbar^2 \frac{\partial}{\partial \eta} \frac{\partial}{\partial \bar{\eta}} - \hbar \frac{eB}{4c} \left( \eta \frac{\partial}{\partial \eta} - \bar{\eta} \frac{\partial}{\partial \bar{\eta}} \right) + \left( \frac{eB}{4c} \right)^2 \eta \bar{\eta} \right] \,,$$

using the coordinate transformation  $\eta = x + iy$ ,  $\bar{\eta} = x - iy$ .

- b) Use the product ansatz  $\psi(\eta, \bar{\eta}) = f(\eta, \bar{\eta}) \exp(-\eta \bar{\eta}/(4l^2))$  with  $l = \sqrt{\hbar c/(eB)}$  and construct the stationary Schrödinger equation for f. Show that the wave function related to the lowest eigenvalue  $E_0 = \hbar \omega_c \ (\omega_c = eB/(\mu c))$  satisfies the condition  $\partial_{\bar{\eta}} f = 0$  and is therefore a polynomial in  $\eta$ .
- c) Calculate the component of the angular momentum operator  $\hat{l}_z$  perpendicular to the x-y plane in complex coordinates  $\eta$  and  $\bar{\eta}$ . Show that  $\left[\hat{\mathcal{H}},\hat{l}_z\right]=0$  and that the functions  $\varphi_m(\eta)=\eta^m\exp(-\eta\bar{\eta}/(4l^2))$  are eigenfunctions of  $\hat{l}_z$ . Calculate their eigenvalues.

Hint: The momentum operator for a charged particle (charge q) in a magnetic field transforms as  $\hat{\mathbf{p}} \to \hat{\mathbf{p}} - \frac{e}{c}\hat{\mathbf{A}}$  with the vector potential for a homogeneous field being  $\mathbf{A} = -\frac{1}{2}(\mathbf{r} \times \mathbf{B})$ . In order to rewrite the partial derivatives in complex coordinates, use the chain rule, e.g., express  $\frac{\partial}{\partial x} f(\eta, \bar{\eta})$  in terms of  $\frac{\partial}{\partial \bar{\eta}}$  and  $\frac{\partial}{\partial \bar{\eta}}$ .

#### IV. ANHARMONIC OSCILLATOR [(12+12+16) PTS]

The Hamiltonian

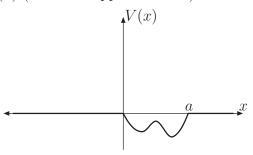
$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_0 + \hat{\mathcal{V}} \equiv \left[ \frac{\hat{p}^2}{2m} + \frac{1}{2} m \omega^2 \hat{x}^2 \right] + \left[ \gamma \hat{x}^4 \right]$$

describes a one-dimensional anharmonic oscillator, where  $\hat{\mathcal{V}}$  is a perturbation of the harmonic oscillator  $\hat{\mathcal{H}}_0$ . As we know the eigenvalues of the harmonic oscillator,  $\hat{\mathcal{H}}_0$ , are  $E_n^{(0)} = \hbar\omega \left(n + \frac{1}{2}\right)$  and the eigenstates can be expressed as  $\left|\psi_n^{(0)}\right> = \frac{1}{\sqrt{n!}}(\hat{a}^\dagger)^n \left|\psi_0^{(0)}\right>$  with the creation (or raising) operator  $\hat{a}^\dagger = (\hat{x}/x_0 + ix_0\hat{p}/\hbar)/\sqrt{2}$  [the corresponding annihilation (or lowering) operator  $\hat{a} = (\hat{x}/x_0 - ix_0\hat{p}/\hbar)/\sqrt{2}$ ] for  $n = 0, 1, 2, \ldots$   $\left[x_0 = \sqrt{\hbar/(m\omega)}\right]$ .  $\hat{a}^\dagger \left|\psi_n^{(0)}\right> = \sqrt{n+1}\left|\psi_{n+1}^{(0)}\right>$  and  $\hat{a} \left|\psi_n^{(0)}\right> = \sqrt{n}\left|\psi_{n-1}^{(0)}\right>$ .

- a) Assuming that  $\gamma$  is small, calculate the ground state energy,  $E_0^{(1)}$ , in first-order perturbation theory.
- b) Calculate the ground state eigenstate,  $\left|\psi_0^{(1)}\right>$ , in first-order perturbation theory.
- c) Calculate the energy eigenvalues in first order perturbation theory for arbitrary n, i.e.,  $E_n^{(1)}$ .

## NIU Physics PhD Candidacy Exam - Spring 2013 - Quantum Mechanics

<u>Problem 1.</u> A particle of mass m and momentum p is incident from the left on a one-dimensional potential well V(x), which is non-zero only between x = 0 and x = a as shown in the figure. The energy  $E = p^2/2m$  of the incident particle is very large compared to the depth of the potential, so that you may treat the potential as small, and keep only effects that are leading order in V(x) (the Born approximation).



- (a) What is  $\phi(x)$ , the unperturbed wavefunction (for V(x) = 0)? [3 points]
- (b) Let us write the perturbed wavefunction as:

$$\psi(x) = \phi(x) + \int_{-\infty}^{\infty} G(x, x') V(x') \phi(x') dx' + \dots$$

Show that G(x, x') then obeys the differential equation

$$\frac{\partial^2}{\partial x^2}G(x,x') + C_1G(x,x') = C_2\delta(x-x')$$

where  $C_1$  and  $C_2$  are positive constants that you will find. [12 points]

(c) Try a solution for G(x, x') of the form:

$$G(x, x') = \begin{cases} Ae^{ik(x-x')} & \text{(for } x \ge x'), \\ Ae^{-ik(x-x')} & \text{(for } x \le x'). \end{cases}$$

Solve for the constants A and k in terms of m and p. [12 points]

(d) Find the probability that the particle will be reflected from the well. Leave your answer in terms of a well-defined integral involving the potential V(x). [13 points]

## Problem 2. Consider the Hamiltonian

$$H = \frac{p^2}{2m} - \alpha \delta(x). \tag{1}$$

Although this problem can be solved exactly, let us approach it variationally and take as a guess for our ground state a Gaussian

$$\psi(x) = Ae^{-bx^2}. (2)$$

- (a) Find the normalization constant A. [8 points]
- (b) Calculate the kinetic energy. [10 points]
- (c) Calculate the potential energy (the delta function). [10 points]
- (d) Find b using the variational principle. [12 points]

#### Problem 3. Consider the three-dimensional infinite cubical well

$$V(x, y, z) = \begin{cases} 0, & \text{if } 0 < x < a, 0 < y < a, 0 < z < a \\ \infty & \text{otherwise} \end{cases}$$

- (a) Find the eigenenergies and eigenstates. [10 points]
- (b) Let us now introduce a perturbation

$$V'(x, y, z) = \begin{cases} V_0, & \text{if } 0 < x < a/2, 0 < y < a/2, 0 < z < a \\ 0 & \text{otherwise} \end{cases}$$

Find the matrix form of V' between the first excited states. [20 points]

(c) Calculate then new eigenenergies and eigenvectors in terms of a and b.[10 points]

<u>Problem 4.</u> Consider a particle of mass m and charge q in a three-dimensional harmonic oscillator described by the Hamiltonian

$$H_0 = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 \, r^2$$

with  $\mathbf{p} = (p_x, p_y, p_z)$  and  $\mathbf{r} = (x, y, z)$ .

(a) Show that the eigenstates of  $H_0$  are eigenstates of angular momentum  $L_z$ . [8 points]

Similarly one can show that the eigenstates of  $H_0$  may also be chosen as eigenstates of angular momentum  $L_x$  and  $L_y$ , so that the eigenstates of  $H_0$  may be labeled  $|n, \ell, m_z\rangle$ , where  $E_n = \hbar \omega (n + \frac{3}{2})$  with n = 0, 1, 2, ... is the eigenvalue of  $H_0$ ,  $\hbar^2 \ell(\ell + 1)$  is the eigenvalue of  $\mathbf{L}^2$  and  $m_z \hbar$  is the eigenvalue of  $L_z$ . We assume that at time  $t = -\infty$  the oscillator is in its ground state,  $|0, 0, 0\rangle$  It is then acted upon by a spatially uniform but time dependent electric field

$$\boldsymbol{\mathcal{E}}(t) = \mathcal{E}_0 \exp(-t^2/\tau^2)\hat{\boldsymbol{z}}$$

(where  $\mathcal{E}_0$  and  $\tau$  are constant).

- (b) Show that, to first order in the perturbation, the only possible excited state the oscillator could end up in is the  $|1,1,0\rangle$  state. [8 points]
- (c) What is the probability for the oscillator to be found in this excited state at time  $t = \infty$ ? [Note that  $\int_{-\infty}^{\infty} \exp[-(x-c)^2] dx = \sqrt{\pi}$  for any complex constant c.] [8 points]
- (d) The probability you obtain should vanish for both  $\tau \to 0$  and  $\tau \to \infty$ . Explain briefly why this is the case. [8 points]
- (e) If instead the oscillator was in the  $|1,1,0\rangle$  state at time  $t=-\infty$ , show that the probability that it ends up in the ground state at time  $t=\infty$  is identical to what was found in part c). [8 points]

# NIU Physics PhD Candidacy Exam - Fall 2012 - Quantum Mechanics

#### Do ONLY THREE out of the four problems. Total points on each problem = 40.

<u>Problem 1.</u> A particle of mass m moves in three dimensions in an attractive potential that is concentrated on a spherical shell:

$$V(\vec{r}) = \begin{cases} -V_0 a \, \delta(r-a) & \text{(for } r=a), \\ 0 & \text{(for } r \neq a), \end{cases}$$

where  $V_0$  is a positive constant with units of energy, and a is a fixed radius and r is the radial spherical coordinate. Consider the lowest bound state of this system with wavefunction denoted  $\psi(\vec{r}) = R(r)/r$  and energy E. Write your answers below in terms of  $\beta \equiv \sqrt{-2mE/\hbar^2}$  and  $a, m, V_0$ .

- (a) Find the Schrödinger differential equation for R(r). [6 points]
- (b) By enforcing proper behavior of the wavefunction at r=0 and  $r=\infty$  and r=a, find the energy of the ground state in terms of the solution to a transcendental equation. [26 points]
- (c) Find the smallest value of  $V_0$  such that there is a bound state. [8 points]

<u>Problem 2.</u> A particle experiences a one-dimensional harmonic oscillator potential. The harmonic oscillator energy eigenstates are denoted by  $|n\rangle$  with  $E_n = (n+1/2)\hbar\omega$ . The state is given by  $|\psi(t)\rangle$ . At t=0, the state describing the particle is

$$|\psi(0)\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$$

- (a) Calculate  $\langle E(t) \rangle = \langle \psi(t) | H | \psi(t) \rangle$  [13 points]
- (b) Calculate  $\langle x(t) \rangle = \langle \psi(t) | x | \psi(t) \rangle$ . [14 points]
- (c) Calculate the root mean squared deviation of x(t). [13 points]

<u>Problem 3.</u> Consider an atomic p electron (l=1) which is governed by the Hamiltonian  $\hat{H} = \hat{H}_0 + \hat{H}_1$  where

$$\hat{H}_0 = \frac{a}{\hbar}\hat{L}_z^2$$
 and  $\hat{H}_1 = \sqrt{2}\frac{c}{\hbar}\hat{L}_x$ ,

with a > 0.

(a) Determine the Hamiltonian  $\hat{H}$  in matrix form for a basis  $|l, m\rangle$ . Restrict yourself to l = 1. You can use the formula

$$\hat{L}_{\pm}|l,m\rangle = \hbar\sqrt{(l\mp m)(l\pm m+1)}|l,m\pm 1\rangle$$
 where  $\hat{L}_{\pm} = \hat{L}_x \pm \hat{L}_y$ .

[14 points]

- (b) We want to treat  $\hat{H}_1$  as a perturbation of  $\hat{H}_0$ . What are the energy eigenvalues and eigenstates of the *unperturbed* problem? [6 points]
- (c) We assume  $a \gg |c|$ . Calculate the eigenvalues and eigenstates of  $\hat{H}$  in second and first order of the perturbation  $\hat{H}_1$ , respectively. [10 points]
- (d) This problem can also be solved exactly. Give the exact eigenvalues and eigenstates and show that they agree with the results obtained in (c). [10 points]

<u>Problem 4.</u> Given the general form of the spin-orbit coupling on a particle of mass m and spin  $\hat{\mathbf{S}}$  moving in a central force potential V(r) is as follows  $(\hat{H}_{SO})$ 

$$\hat{H}_{SO} = \frac{1}{2m^2c^2}\hat{\mathbf{L}} \cdot \hat{\mathbf{S}} \frac{1}{r} \frac{dV(r)}{dr}$$

Assume a electron (s = 1/2) in the central force potential V(r) of a spherically symmetric 3D simple harmonic oscillator,

- (a) Evaluate  $\langle \hat{H}_{SO} \rangle$ . [20 points]
- (b) What is the energy shift for those states with  $\ell=0$ ? [10 points]
- (c) What are the possible j for those states with  $\ell=1$ ? [5 points]
- (d) Evaluate the energy shift for those states with  $\ell=1$  [5 points]

# NIU Physics PhD Candidacy Exam – Spring 2012 – Quantum Mechanics DO ONLY THREE OUT OF FOUR QUESTIONS

#### Problem 1.

Assume that the lowest-energy eigenfunction of the simple harmonic oscillator is approximated by

$$u_0(x) = N \exp(-ax^2), \tag{1}$$

where a is the constant we want to determine and N is a normalization constant.

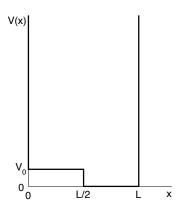
- (a) Determine the normalization constant N. See also the integrals at the end of the question. [8 points]
- (b) Calculate the energy in terms of a and the angular frequency  $\omega$ . [12 points]
- (c) Determine a by minimizing the energy with respect to a. [10 points]
- (b) Determine the energy associated with the lowest eigenfunction. [10 points]

$$\int_0^\infty e^{-\alpha x^2} dx = \frac{1}{2} \sqrt{\frac{\pi}{\alpha}} \quad \text{and} \quad \int_0^\infty x^2 e^{-\alpha x^2} dx = \frac{1}{4\alpha} \sqrt{\frac{\pi}{\alpha}}$$
 (2)

#### Problem 2.

A particle of mass m is confined to an infinitely high one-dimensional potential box of width L. At the bottom of the box, there is a bump in the potential of height  $V_0$  and width L/2, as shown.

- (a) Find the ground-state wavefunction to first order in perturbation theory in  $V_0$ . [18 points]
- (b) Find the ground-state energy to second order in perturbation theory in  $V_0$ . [16 points]
- (c) What condition must hold for the perturbation expansion to make sense? Give the answer in terms of  $V_0$ , m, L, and  $\hbar$ . [6 points]



## Problem 3.

The first excited state of a three-dimensional isotropic harmonic oscillator (of natural angular frequency  $\omega_0$  and mass m) is three-fold degenerate.

- (a) Calculate to first order the energy splittings of the three-fold degenerate state due to a small perturbation of the form H' = bxy where b is a constant. [25 points]
- (b) Give the first-order wavefunction of those three levels in terms of the wavefunctions of the unperturbed three-dimensional harmonic oscillator. [15 points]

Hint: For a one-dimensional harmonic oscillator

$$\langle n|x|n+1\rangle = \sqrt{\frac{\hbar(n+1)}{2m\omega_0}}.$$
 (3)

#### Problem 4.

(a) Consider a spherical potential well with

$$U(r) = 0 r < a ; U(r) = \infty r > a (4)$$

Give the radial part of the Schrödinger equation for r < a. [10 points]

- (b) We are now only interested in the wavefunction for l = 0. Give the general solution of the differential equation by trying a solution for the radial part of the wavefunction R(r) = P(r)/r. (Normalization is not necessary). [10 points]
- (c) Determine the behavior of the wavefunction for  $r \to 0$ . What does the condition that the wavefunction should not diverge at r = 0 imply? [10 points]
- (d) Determine the energy eigenvalues for l = 0. [10 points]

# PhD Qualifying Exam Fall 2011 – Quantum Mechanics Do only 3 out of the 4 problems

<u>Problem 1.</u> A spinless, non-relativistic particle of mass m moves in a three-dimensional central potental V(r), which vanishes for  $r \to \infty$ . The particle is in an exact energy eigenstate with wavefunction in spherical coordinates:

$$\psi(\vec{r}) = Cr^n e^{-\alpha r} \sin(\phi) \sin(2\theta),$$

where C and n and  $\alpha$  are positive constants.

- (a) What is the angular momentum of this state? Justify your answer. [10 points]
- (b) What is the energy of the particle, and what is the potential V(r)? [30 points]

<u>Problem 2.</u> Apply the variational principle to the anharmonic oscillator having the Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + Cx^4. \tag{1}$$

(a) Use as your trial wavefunction a form that is similar to the wavefunction for a harmonic oscillator:

$$\psi(x) = \left(\frac{\lambda^2}{\pi}\right)^{1/4} e^{-\frac{\lambda^2 x^2}{2}} \tag{2}$$

to determine the variational constant  $\lambda$  that minimizes the expectation value of  $\hat{H}$ . Note:  $\int_{-\infty}^{\infty} e^{-ax^2} dx = \sqrt{\pi/a}.$  [25 points]

(b) The ground state energy of the anharmonic oscillator using numerical methods is

$$E_0 = 1.060 \left(\frac{\hbar^2}{2m}\right)^{2/3} C^{1/3}. \tag{3}$$

What is the approximate ground state energy using the variational method? How does it compare to the numerical results? [15 points]

<u>Problem 3.</u> The eigenstates of the hydrogen atom are perturbed by a constant uniform electric field E which points along the z direction. The perturbation is given by

$$H' = -eEz = -eEr\cos\theta. \tag{4}$$

The eigenstates  $\psi_{nlm}(\mathbf{r})$  are  $n^2$ -fold degenerate for a particular n. The electric field lifts this degeneracy. Let us consider n=2.

- (a) Write down the hydrogen wavefunctions for n=2 when H'=0. [5 points]
- (b) Only two matrix elements of H' between the different states for n=2 are nonzero. Explain why the other diagonal and off-diagonal matrix elements are zero. [5 points]
- (c) Evaluate the matrix elements by using the expressions for the wavefunctions below and in the formula sheet. You do not have to evaluate the integral over the radial coordinate r (or  $\rho = r/a_0$ , where  $a_0$  is the Bohr radius). [15 points]
- (d) Find the eigenenergies and eigenfunctions for the n=2 levels in the electric field. [15 points]

Additional information:

For Z = 1 and n = 2, we have

$$R_{20} = \frac{1}{(2a_0)^{3/2}} (2 - \rho) e^{-\rho/2}$$
 and  $R_{21} = \frac{1}{\sqrt{3}(2a_0)^{3/2}} \rho e^{-\rho/2}$ , (5)

with  $\rho = r/a_0$ , where  $a_0$  is the Bohr radius.

<u>Problem 4.</u> A free electron is at rest in a uniform magnetic field  $\vec{B} = \hat{x}B$ . The interaction Hamiltonian is

$$H = k\vec{S} \cdot \vec{B}$$
,

where k is a constant. At time t = 0, the electron's spin is measured to be pointing in the  $+\hat{z}$  direction.

- (a) What is the probability that at time t = T the electron's spin is measured to point in the  $-\hat{z}$  direction? [25 points]
- (b) What is the probability that at time t = T the electron's spin is measured to point in the  $+\hat{x}$  direction? [15 points]

# NIU Physics PhD Candidacy Exam – Spring 2011 – Quantum Mechanics DO ONLY THREE OUT OF FOUR QUESTIONS

#### Problem 1.

- (a) In general, what is the first order correction to the energy of a quantum state for a one dimensional system with a time independent perturbation given by H'? [8 points]
- (b) Suppose in an infinite square well between x = 0 and x = a the perturbation is given by raising one half of the floor of the well by  $V_0$ ? What is the change in energy to the even and to the odd states? [16 points]
- (c) Now suppose the perturbation is given by  $\alpha\delta(x-a/2)$  where  $\alpha$  is constant. What is the first order correction to the allowed energies for the even and odd states? [16 points]

#### Problem 2.

We consider scattering off a spherical potential well given by

$$V(r) = \begin{cases} -V_0 & r \le a \\ 0 & r > a \end{cases} \qquad V_0, a > 0$$

The particle's mass is m. We restrict ourselves to low energies, where it is sufficient to consider s wave scattering (angular momentum l = 0).

- (a) Starting from the Schrödinger equation for this problem, derive the phase shift  $\delta_0$ . [14 points]
- (b) Calculate the total scattering cross section  $\sigma$  assuming a shallow potential well  $(a\sqrt{2mV_0/\hbar^2}\ll 1)$ . [ 10 points ]
- (c) Show that the same total scattering cross section  $\sigma$  as in b) is also obtained when using the Born approximation. Note: part c) is really independent of parts a) and b). [16 points]

#### Problem 3.

For a quantum harmonic oscillator, we have the position  $\hat{x}$  and momentum  $\hat{p}_x$  operators in terms of step operators

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

giving a Hamiltonian  $H = \hbar\omega(a^{\dagger}a + \frac{1}{2})$ .

- (a) The eigenstates with energy  $(n + \frac{1}{2})\hbar\omega$  in bra-ket notation are  $|n\rangle$ . Express the eigenstates in terms of the step operators and the state  $|0\rangle$  (no need to derive). [8 points]
- (b) Show that the eigenstates  $|1\rangle$  and  $|2\rangle$  are normalized using the fact that  $|0\rangle$  is normalized (or derive the normalization factor for those states, in case your result from (a) is not normalized). [8 points]
- (c) Calculate the expectation values of  $\langle \hat{x}^2 \rangle$  and  $\langle \hat{p}_x^2 \rangle$  for the eigenstates  $|n\rangle$ . [8 points]
- (d) Using the result from (c), show that the harmonic oscillator satisfies Heisenberg's uncertainty principle (consider only eigenstates). [8 points]
- (e) The term  $H' = \gamma x^2$  is added to the Hamiltonian. Find the eigenenergies of H + H'. [8 points]

# Problem 4.

- (a) We want to study the spin-orbit coupling for an atomic level with l=2. How will this level split under the interaction  $\zeta \mathbf{L} \cdot \mathbf{S}$ ? Give also the degeneracies. [8 points]
- (b) Show that for an arbitrary angular momentum operator (integer and half-integer), we can write

$$J_{\pm}|jm_{j}\rangle = \sqrt{(j \mp m_{j})(j \pm m_{j} + 1)}|jm_{j} \pm 1\rangle \tag{2}$$

(take  $\hbar = 1$ ) [Hint: Rewrite  $J_{\pm}J_{\mp}$  in terms of  $J^2$  and  $J_z$ ]. [10 points]

- (c) Since  $m_j$  is a good quantum number for the spin-orbit coupling, we can consider the different  $m_j$  values separately. Give the matrix for  $\zeta \mathbf{L} \cdot \mathbf{S}$  in the  $|lm, \frac{1}{2}\sigma\rangle$  basis with  $\sigma = \pm \frac{1}{2}$  for  $m_j = 3/2$ . Find the eigenvalues and eigenstates of this matrix. [12 points]
- (d) Write down the matrix for the spin-orbit coupling in the  $|jm_j\rangle$  basis for  $m_j=3/2$ . [10 points]