Quantum Mechanics
Qualifying Exam - August 2018

Notes and Instructions

- There are 6 problems. Attempt them all as partial credit will be given.
- Write on only one side of the paper for your solutions.
- Write your alias on the top of every page of your solutions.
- Number each page of your solution with the problem number and page number (e.g. Problem 3, p. 2/4 is the second of four pages for the solution to problem 3.)
- You must show your work to receive full credit.

Possibly useful formulas:

Spin Operator

$$\vec{S} = \frac{\hbar}{2}\vec{\sigma}, \quad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{1}$$

In spherical coordinates,

$$\nabla^2\psi = \frac{1}{r}\frac{\partial^2}{\partial r^2}r\psi + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial\psi}{\partial\theta}) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\psi. \tag{2}$$

Harmonic oscillator wave functions

$u_0(x) = (\frac{m\omega}{\pi\hbar})^{1/4}e^{-\frac{m\omega x^2}{2\hbar}}$

$u_1(x) = (\frac{m\omega}{\pi\hbar})^{1/4}\sqrt{\frac{2m\omega}{\hbar}}xe^{-\frac{m\omega x^2}{2\hbar}}$

Problem 1: Hilbert Spaces, Matrix Mechanics (10 pts)

A system is made up of two spins, spin 1 and spin 2. The system is described in the basis $|uu\rangle$, $|ud\rangle$, $|du\rangle$, and $|dd\rangle$, where "u" and "d" stand for "up" and "down", the first entry denotes the state of spin 1, and the second entry denotes the state of spin 2. The Hamiltonian is

$$\hat{H} = E_0 + \frac{\lambda}{4}\hat{\sigma}_1 \cdot \hat{\sigma}_2 = E_0 + \frac{\lambda}{4}(\hat{\sigma}_{1x}\hat{\sigma}_{2x} + \hat{\sigma}_{1y}\hat{\sigma}_{2y} + \hat{\sigma}_{1z}\hat{\sigma}_{2z}) \; . \tag{1}$$

In the above equation, E_0 is a constant and λ is the strength of the coupling between the spins. The σ_{ix}, σ_{iy}, and σ_{iz} denote the usual Pauli matrices with $i = 1, 2$.

Initially at time $t = 0$, the system is in the state $|\psi(0)\rangle = \alpha\,|uu\rangle + \beta\,|ud\rangle$, normalized so that $|\alpha^2| + |\beta|^2 = 1$.

a) (7pts) Represent the Hamiltonian $\hat{H}$ as a matrix in the given basis.

b) (0.5pts) Find the eigenbasis of $\hat{H}$.

c) (0.5pts) Express $|\psi(0)\rangle$ in terms of the eigenbasis of $\hat{H}$.

d) (2pts) Calculate $|\psi(t)\rangle$ at a later time t.

Problem 2: Two State System (10 pts)

In this problem, we will consider a two state system defined by the Hamiltonian

$$\tilde{\mathbf{H}} = |1\rangle\langle 1| + i\sqrt{3}\,|2\rangle\langle 1| + c\,|1\rangle\langle 2| - |2\rangle\langle 2|$$

in the basis set $\{|1\rangle, \ |2\rangle\}$.

a) (2pts) What is the numerical value of c? Explain.

b) (4pts) Calculate the eigenvalues and the associated properly normalized eigenstates for this Hamiltonian. Express the eigenstates in Dirac notation.

c) (4pts) If a system described by this Hamiltonian is initially in the state $|\psi\rangle = |1\rangle$, calculate the probability that the system will be in the state $|2\rangle$ at a later time t.

Problem 3: L=1 system (10 pts)

Consider the following operators on a 3-dimensional Hilbert space ($\hbar = 1$).

$$L_x = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad L_y = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad L_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

a) (1pt) What are the possible values one can obtain if L_z is measured?

b) (1pt) Take the state in which $\langle L_z \rangle$=1. In this state, determine $\Delta L_x = \sqrt{\langle L_x^2 \rangle - \langle L_x \rangle^2}$

c) (2pts) Find the normalized eigenstates and eigenvalues of L_x in the L_z basis.

d) (2pts) If the particle is in the state with $\langle L_z \rangle$=-1 and L_x is measured, what are the possible outcomes and their probabilities?

e) (2pts) Consider the state

$$|\psi\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \\ 1 \end{pmatrix},$$

in the L_z basis. If L_z^2 is measured and a result of +1 is obtained, what is the state after the measurement. How probable was this result? If L_z is measured, what are the outcomes and respective probabilities?

f) (2pts) Write down the most general normalized state for which the probabilities are P($\langle L_z \rangle$=1)=1/4, P($\langle L_z \rangle$=0)=1/2 and P($\langle L_z \rangle$=-1)=1/4 including phase angles.

Write this state in the L_x basis and determine the probability that $\langle L_x \rangle$=0, to show that relative phases can affect the probability.

Problem 4: Coulomb interaction (10 pts)

Where appropriate, make sure that the wave function has the proper symmetry under the exchange of identical particles.
This problem treats the nucleus as an infinitely heavy positively charged point particle. The only interaction at play is the Coulomb interaction. Electrons are treated as spin-1/2 particles and relativistic effects are neglected.

a) (2pts) What are the eigen energies of the hydrogen atom, He^+ ion, and C^{5+}?

   Compare the "sizes" of the ground state of these three systems.

b) (2pts) Neglecting the electron-electron repulsion, what are the ground state energy and ground state wave function of the (neutral) helium-atom? In addressing this question, consider the spatial and spin degrees of freedom of the electrons.

c) (3pts) Neglecting the electron-electron repulsion, construct the excited state wave functions and associated energy spectrum of the (neutral) helium atom. Explicitly comment on the roles of "spin singlet" and "spin triplet".

d) (3pts) Neglecting electron-electron interactions, what is the ground state wave function of the neon atom? Make sure to explain what you are doing.

Problem 5: Wave functions, uncertainty, and potential (10 pts)

Consider the time-independent, one-dimensional wave function $\psi(x) = ce^{-ax^2}$, where a and c are real constants. You may find the following integrals useful for this problem:

$$\int_{-\infty}^{\infty} e^{-bx^2} dx = \sqrt{\frac{\pi}{b}} \tag{2}$$

$$\int_{-\infty}^{\infty} x^2 e^{-bx^2} dx = \frac{1}{2}\sqrt{\frac{\pi}{b^3}} \tag{3}$$

a) (2pts) Determine the value of c such that this wave function is properly normalized.

b) (3pts) Calculate $< x >$, $< x^2 >$, $< p_x >$, and $< p_x^2 >$.

c) (3pts) What is the value of the product of the uncertainties on x and p_x, $\Delta x \Delta p_x$? Does this state abide by Heisenberg's uncertainty principle? Explain why or why not.

d) (2pts) Find the potential profile $U(x)$ for which this wave function is a solution. If need be, shift the potential by a constant to put it into a more recognizable form. What physical problem does this wave function correspond to? Define a in terms of more fundamental constants?

Problem 6: x^4 Simple Harmonic Oscillator Perturbation (10 pts)

(Note this problem is 2 pages and has 6 parts)

Consider a Simple Harmonic Oscillator described by the Hamiltonian,

$$H_0 = \frac{p^2}{2} + \frac{x^2}{2} \tag{4}$$

This Hamiltonian comes from the choice of units $m = \omega = \hbar = 1$. In these units, the properties of the SHO can be defined using:

$$H_0|n\rangle = \left(n + \frac{1}{2}\right)|n\rangle, \quad n = 0, 1, 2, 3, ... \tag{5}$$

$$\hat{a} = \frac{1}{\sqrt{2}}(x + ip), \quad \hat{a}^\dagger = \frac{1}{\sqrt{2}}(x - ip), \quad \hat{n} = \hat{a}^\dagger\hat{a}, \quad H_0 = \hat{n} + \frac{1}{2} \tag{6}$$

Also, because of the units being used,

$$p = i\frac{\partial}{\partial x}, \quad [x, p] = i, \quad \left[\hat{a}, \hat{a}^\dagger\right] = 1, \quad \left[\hat{n}, \hat{a}^\dagger\right] = \hat{a}^\dagger, \quad [\hat{n}, \hat{a}] = -\hat{a} \tag{7}$$

In terms of wavefunctions:

$$\psi_n(x) = \frac{1}{\pi^{1/4}}\left(\frac{1}{2^n n!}\right)^{1/2}\mathcal{H}_n(x)e^{-\frac{1}{2}x^2}. \tag{8}$$

where $\mathcal{H}_n(x)$ are the Hermite Polynomials.

The simplest, non-trivial, physical perturbation to this Hamiltonian is proportional to x^4, giving the perturbed Hamiltonian:

$$H' = H_0 + H_1 = H_0 + \gamma x^4 \tag{9}$$

a)[2 pts.] Calculate the result of operating with the perturbative potential on the ground state: $H_1|0\rangle = \gamma x^4|0\rangle$.
Your answer should be a sum (expansion) in terms of the states $|n\rangle$.

b)[2 pts.] Using your result from (b) (or any other way you wish to do this) calculate the first order correction, in γ, to the ground state of H_0.

c)[2 pts] Using your result from (b) (or any other way you wish to do this) calculate the second order correction, in γ, to the ground state of H_0.

d)[1 pt.] Show that for *any* quantum state, $|\psi\rangle$,

$$\langle\psi|H_0|\psi\rangle \geq \frac{1}{2}. \tag{10}$$

Problem 6 continued

The result from (d) is used in the variational approximation, where the ground state energy can be approximated by minimizing the expectation value of the Hamiltonian using a set of trial wavefunctions that might approximate the correct ground-state wavefunction.

e) [2 pts.] Use a trial wavefunction of the form

$$\psi(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\frac{\alpha}{2}x^2} \tag{11}$$

and the variational method to approximate the ground state energy of the perturbed Hamiltonian H'.

In this problem, derive an expression for the best value of α for determining the approximate ground state energy, but do not actually attempt to solve this expression exactly.

f) [1 pt.] Compare your variational result in the limit $\gamma \to 0$ to your results from question (b). Explain any similarities and differences between the variational result and the perturbation results.

An integral you might wish to use for solving this problem is:

$$\int_{-\infty}^{\infty} x^{2n} e^{-\alpha x^2} dx = \sqrt{\frac{\pi}{\alpha}} \frac{(2n-1)!!}{2^n \alpha^n} \tag{12}$$

where for an integer $n > 0$, $(2n-1)!! = (2n-1)(2n-3)...(3)(1)$ and for an integer $n \leq 0$, $(2n-1)!! = 1$.