Quantum Mechanics
Qualifying Exam - Spring 2023

Notes and Instructions

- There are 6 problems. Attempt them all as partial credit will be given.
- Write your alias on the top of every page of your solutions. *Do not write your name.*
- 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 all your work to receive full credit.

Possibly useful formulas:

Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Laplacian in spherical coordinates

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

One dimensional simple harmonic oscillator operators:

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

Spherical Harmonics:

$$\begin{aligned}
Y_0^0(\theta,\phi) &= \frac{1}{\sqrt{4\pi}}, \\
Y_1^0(\theta,\phi) &= \sqrt{\frac{3}{4\pi}}\cos\theta \\
Y_1^{\pm1}(\theta,\phi) &= \mp\sqrt{\frac{3}{8\pi}}\sin\theta \mathbf{e}^{\pm i\phi} \\
Y_2^0(\theta,\phi) &= \sqrt{\frac{5}{16\pi}}(3\cos^2\theta - 1) \\
Y_2^{\pm1}(\theta,\phi) &= \mp\sqrt{\frac{15}{8\pi}}(\sin\theta\cos\theta)\,\mathbf{e}^{\pm i\phi} \\
Y_2^{\pm2}(\theta,\phi) &= \sqrt{\frac{15}{32\pi}}\sin^2\theta\,\mathbf{e}^{\pm 2i\phi}
\end{aligned}$$

PROBLEM 1: Hydrogen atom

The normalized wavefunction of an electron in the ground state ($1s$) of hydrogen is given by

$$\psi(r) = \sqrt{\frac{1}{\pi a_0^3}} e^{-r/a_0},$$

where $a_0 \approx 0.529$ nm is the Bohr radius. Assuming that the given wave function is valid at $r = 0$, there is a nonzero probability of finding the electron within the nucleus.

a) If the nuclear volume has radius $r = b$, derive an exact expression for the probability of finding the electron within the nucleus. (3 points)

b) Calculate the radial expectation value of the electron, $\langle r \rangle$, and compare this to the approximate size of the nucleus ($b \approx 10^{-15}$ m). (3 points)

c) Compare your result in (a) to that obtained by assuming the wavefunction has a constant value of $\psi(0)$ within the nuclear volume. (Hint: expand your result in (a) assuming $b \ll a_0$) (3 points)

d) What is the electronic charge density in the nuclear region and hence the fractional electronic charge that would be within the nucleus? (1 point)

PROBLEM 2: Hilbert Space

Consider a quantum system described by a 3-dimensional Hilbert space with a Hamiltonian $\hat{H}$ and two observables $\hat{A}$ and $\hat{B}$:

$$\hat{H} = \hbar\omega \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad \hat{A} = a \begin{pmatrix} 0 & i & 0 \\ -i & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \hat{B} = b \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \tag{1}$$

These operators are defined using the eigenvectors of the Hamiltonian as a basis, $|e_j\rangle$, $j = 1, 2, 3$ with

$$\hat{H}|e_1\rangle = \hbar\omega|e_1\rangle, \quad \hat{H}|e_2\rangle = \hbar\omega|e_2\rangle, \quad \hat{H}|e_3\rangle = -\hbar\omega|e_3\rangle \tag{2}$$

a) Show that the eigenvalues of $\hat{A}$ are $\pm a$ and the eigenvalues of $\hat{B}$ are $\pm b$. (1 point)

b) Derive an orthonormal set of eigenvectors for $\hat{A}$ and an orthonormal set of eigenvectors for $\hat{B}$. (2 points)

c) At time $t = 0$, the system is in the state $|e_2\rangle$ when $\hat{B}$ is measured. What are the probabilities of measuring b and $-b$? Show your work. (2 points)

d) Let the result of the measurement in part c) be $-b$. The system is then allowed to propagate until a time $t > 0$ when a measurement of $\hat{A}$ is made. What is the probability to find the result $-a$? (2 points)

e) Instead of the measurement of $\hat{A}$, after measuring $\hat{B}$ with result $-b$ at $t = 0$, a measurement of $\hat{B}$ is made at $t > 0$. What is the probability to find the result $-b$? (2 points)

f) Explain the difference in the time-dependence of the results from parts d) and e). (1 point)

PROBLEM 3: Harmonic Oscillator

The Hamiltonian $\hat{H}$ for the 1d harmonic oscillator with mass m and angular frequency ω can be written in terms of the position operator $\hat{x}$ and momentum operator $\hat{p}$,

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

a) Starting from the representation-independent eigenvalue equation

$$\hat{H}|a_E\rangle = E|a_E\rangle,$$

where $|a_E\rangle$ denotes an energy eigenket of the 1d harmonic oscillator with eigenenergy E, derive the time-independent Schrödinger equation

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x'^2} + \frac{1}{2}m\omega^2 x'^2\right)\psi_{a_E}(x') = E\psi_{a_E}(x').$$

You may use:

- $\hat{x}|x'\rangle = x'|x'\rangle$,
- $\hat{p}|p'\rangle = p'|p'\rangle$,
- $\langle x'|p'\rangle = (2\pi\hbar)^{-1/2}\exp(\imath x'p'/\hbar)$,
- $\langle x''|x'\rangle = \delta(x'' - x')$,
- $\int dp'|p'\rangle\langle p'| = \hat{1}$,
- $\int dx'|x'\rangle\langle x'| = \hat{1}$, and
- $\langle x'|a_E\rangle \equiv \psi_{a_E}(x')$

(4 points).

b) Using the energy eigenkets $|a_E\rangle$ of the harmonic oscillator, write down their completeness relation. State carefully what, if anything, is being summed over and how many, if any, terms there are in the sum. (1.5 points)

c) Starting with your answer to part (b), rewrite the completeness (closure) relation in terms of $\psi_{a_E}(x')$. (1.5 points)

d) The density of states is defined as the number of states per unit energy interval. How does the density of states of the 1d harmonic oscillator change with energy, i.e., does it increase, does it decrease, or does it stay constant with increasing energy? Explain your answer. You do not have to worry about proportionality factors to answer this question. (1.5 points)

e) How does the density of states of the isotropic 3d harmonic oscillator change with energy, i.e., does it increase, does it decrease, or does it stay constant with increasing energy? Explain your answer. Again, you do not have to worry about proportionality factors to answer this question. (1.5 points)

PROBLEM 4: Central Potential

The deuteron is a bound state of a proton and a neutron. It may be described crudely by a spherical square well of depth $V_0 > 0$ and range a:

$$U(r) = \begin{cases} -V_0 & r < a \\ 0 & \text{otherwise}\,. \end{cases}$$

The radial Schrödinger equation is given by

$$\left[-\frac{\hbar^2}{2\mu r^2} \frac{d}{dr}\left(r^2 \frac{d}{dr} \right) + \frac{\hbar^2 \ell(\ell+1)}{2\mu r^2} + U(r) \right] R(r) = E R(r)\,,$$

where μ is the reduced mass of a deuteron, ℓ is the orbital angular momentum quantum number and E is the energy of a bound state ($-V_0 \leq E \leq 0$).

a) By substituting $R(r) = u(r)/r$, determine the form of physically allowed (normalizable) s-wave ($\ell = 0$) solution $u(r)$ *inside the well*. (2 points)

b) Do the same as in part a), but *outside the well*. (2 points)

c) By matching $d(\ln u)/dr$ at $r = a$, derive a transcendental equation relating the allowed wave numbers in both regions. (3 points)

d) Assume that a bound state exists with $|E| \ll V_0$. Solve the equation from c) in the limit $E \to 0$ to determine the value of the dimensionless quantity $\sqrt{2\mu V_0/\hbar^2}\,a$. (3 points)

PROBLEM 5: Angular Momentum Theory

Suppose we have a system with two angular momentum operators $\vec{J}_1$ and $\vec{J}_2$, each with Hilbert spaces spanned by the $\{|j_1, m_1\rangle\}$ and $\{|j_2, m_2\rangle\}$ basis respectively, with j_1, j_2 the angular momentum quantum numbers and m_1, m_2 the magnetic quantum numbers. The total angular momentum operator is given by $\vec{J} = \vec{J}_1 + \vec{J}_2$, which acts in the Hilbert space spanned by the $\{|j, m\rangle\}$ basis.

a) What are the basis states in the direct product basis between the Hilbert spaces of $\vec{J}_1$ and $\vec{J}_2$? List them as ket-vectors. (1 point)

b) List the good (diagonal) operators in the direct product basis along with their eigenvalues. (1 point)

c) What is the completeness (closure) relation for the direct product basis states of part a)? (1 point)

d) What are the good (diagonal) operators in the total angular momentum basis $\{|j, m\rangle\}$ and what are their eigenvalues? (1 point)

e) Write a relationship between the total angular momentum basis states $|j, m\rangle$ and the direct product basis states. (2 points)

f) Suppose $j_1 = \frac{1}{2}$ and $j_2 = 1$. How do the direct product basis states break up into irreducible representations, *i.e.* what is $\frac{1}{2} \otimes 1$ equal to? (2 points)

g) How are the quantum numbers in each irreducible representation you found in part f) related to product state quantum numbers? (2 points)

PROBLEM 6: Perturbation Theory

A system with discrete energy levels has the Hamiltonian $H = H_0 + \lambda H'$. Assume that the dimensionless parameter $|\lambda| \ll 1$, H_0 and H' are time independent, with

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

and

$$H|\psi_n\rangle = E_n|\psi_n\rangle.$$

Assume also that H_0 is *non-degenerate* and that the eigenstates and eigenkets of the perturbed Hamiltonian H can be expanded in powers of the parameter λ as

$$E_n = \sum_{m=0}^{\infty} \lambda^m E_n^{(m)}, \qquad |\psi_n\rangle = \sum_{m=0}^{\infty} \lambda^m |\psi_n^{(m)}\rangle,$$

where $E_n^{(m)}$ and $|\psi_n^{(m)}\rangle$ are the m-th order corrections to the energy and eigenkets due to the perturbation H'.

a) *Derive* the first order energy correction $E_n^{(1)}$ due to the perturbation H'. Express your answer in terms of unperturbed eigenkets. Show all your work. (2 points)

b) As in part a), *derive* the second order energy correction $E_n^{(2)}$. Express your answer in terms of unperturbed eigenenergies and eigenkets. Show all your work. (2 points)

Now consider a particle with charge q in a one-dimensional harmonic oscillator potential described by the Hamiltonian

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

where $\hat{x}$ is the coordinate operator and $\hat{p}$ the momentum operator. An external electric field E is applied in the positive x direction which adds to H_0 the potential $V(x) = -qE\hat{x}$.

c) Use perturbation theory to calculate the first order energy shifts in the energy levels. (1 point)

d) Use perturbation theory to calculate the second order energy shifts in the energy levels. (2 points)

e) This problem can be solved exactly. Find the exact eigenvalues and compare them with the perturbative result above. (3 points)