Quantum Mechanics
Qualifying Exam - August 2021

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:

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

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: Time-dependent Quantum States

Consider a particle of mass m in a 1D infinite square well of width L:

$$V(x) = \begin{cases} 0, & |x| \le L/2 \\ \infty, & |x| > L/2 \end{cases}.$$

a) Solve for the normalized, *time-dependent* energy eigenfunctions of the particle, $\Psi_n(x,t)$, where n is an integer. Show your work. (2 points)

b) Calculate the time-dependent expectation value of the position of the particle in the states found in part a), $\langle \Psi_n | x | \Psi_n \rangle(t)$. Explain why your result makes physical sense. (1 point)

c) Let us define the states

$$\Phi_n(x,t) = \frac{1}{\sqrt{2}} \left(\Psi_n(x,t) + \Psi_{n+1}(x,t) \right),$$

with n an odd integer ($n = 1$ is the ground state). Write down, using Dirac notation, an expression for the time-dependent expectation value: $\langle x \rangle_n(t) = \langle \Phi_n(t) | x | \Phi_n(t) \rangle$. Simplify this expression as much as possible without doing any integrals to determine the time dependence of the expectation value of x. (2 points)

d) Determine the oscillation frequency of $\langle x \rangle_n(t)$ as a function of n and the physical parameters in the problem. (1 point)

e) How would your answers to parts c) and d) change if the states were re-defined as

$$\tilde{\Phi}_n(x,t,\eta) = \frac{1}{\sqrt{2}} \left(\Psi_n(x,t) + e^{i\eta} \Psi_{n+1}(x,t) \right),$$

with η a real constant? (1 point)

f) Solve for the amplitude of the expectation value: $\langle x \rangle_n(t) = \langle \tilde{\Phi}_n(t) | x | \tilde{\Phi}_n(t) \rangle$. Does this amplitude get larger, smaller, or stay the same as n gets larger? (3 points)

You might find the following integrals useful:

$$\int x \sin(ax)\, dx = \frac{1}{a^2} \sin(ax) - \frac{x}{a} \cos(ax)$$

$$\int \cos^2(x)\, dx = \frac{1}{2} \left(x + \sin(x) \cos(x) \right)$$

$$\int \sin^2(x)\, dx = \frac{1}{2} \left(x - \sin(x) \cos(x) \right)$$

PROBLEM 2: Spin $\frac{1}{2}$ mechanics

Consider a two-component spinor given in the z-basis by

$$|\chi\rangle = \begin{pmatrix} e^{i\alpha/2}\cos(\beta/2) \\ e^{-i\alpha/2}\sin(\beta/2) \end{pmatrix},$$

where α and β are real parameters. For a 2-level system, the rotation matrix about $\hat{n}$ by an angle θ, is given by

$$U_R = \mathbf{I}\cos(\theta/2) - i\hat{n}\cdot\vec{\sigma}\sin(\theta/2),$$

where $\mathbf{I}$ is the identity matrix, and $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$, the vector composed of the Pauli spin matrices.

a) What is the probability for χ to be found in the state

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

as a function of β? (2 points)

b) Suppose you apply U_R to $|\chi\rangle$ by an amount $\theta = \Omega t$ about $\hat{n} = \hat{y}$. What is the probability to observe $|1\rangle$ as a function of t? (3 points)

c) Find one value of α for which the rotation in (b) can achieve perfect polarization in the z-basis, i.e., either $|1\rangle$ or

$$|2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix},$$

for specific values of Ωt. (2 points)

d) Propose an operator $\hat{U}$ mapping χ to $|1\rangle$ or equivalently $\hat{U}\chi = |1\rangle$ for any α and β. **Hint:** This could be the product of $\hat{z}$ and $\hat{y}$ rotations suggested by part (c). (3 points)

PROBLEM 3: Quantum rotor

Consider an electrically-charged particle constrained (confined) to move along the perimeter of a circle with radius R. This particle has just one degree of freedom, say the displacement arc $\ell = R\phi$. So, its energy (and Hamiltonian) is similar to that of a free 1D particle (with the replacement $x \to \ell$):

$$\hat{\mathcal{H}} = \frac{\hat{p}^2}{2m} \quad \text{with } \hat{p} = -i\hbar\frac{\partial}{\partial \ell}$$

The eigenfunctions also have a similar structure: $\psi = Ce^{ik\ell}$.

a) Using the proper boundary condition, find the allowed energies E_n of the particle. (2 points)

b) What are the (normalized) stationary states? (1 point)

c) Calculate explicitly the expectation value for the momentum of the particle in the nth stationary state. (2 points)

d) The particle is prepared to be in the state:

$$\psi(\phi) = \frac{1}{\sqrt{4\pi}}\left(1 + e^{i\phi}\right)$$

What is the expectation value of the particle's energy? (2 points)

e) A uniform magnetic field is applied, with a magnitude of B, directed perpendicular to plane of motion. In this case, the Hamiltonian becomes:

$$\hat{\mathcal{H}} = \frac{1}{2m}\left(-ih\hat{\phi}\frac{\partial}{\partial \ell} - q\vec{A}\right)^2$$

where we can take:

$$\vec{A} = \hat{\phi}\frac{BR}{2}$$

What are the allowed energies E_n of the particle? (3 points)

PROBLEM 4: Free particle in 1D

A free particle moves in 1D. At $t = 0$ the normalized wavefunction is

$$\psi(x,0) = \left(\frac{\alpha}{\pi}\right)^{1/4} \mathrm{e}^{ik_0 x - \alpha x^2/2},$$

where $\alpha > 0$ and k_0 is a real parameter.

a) Find the momentum wavefunction $\psi(k,t)$ at all times $t > 0$ and the momentum probability density $\mathcal{P}(k,t)$. What is the most probable momentum? (2 points)

b) Compute the wavefunction $\psi(x,t)$ at all times $t > 0$ and the corresponding probability density $\mathcal{P}(x,t)$. How does the most probable position evolve in time? (3 points)

c) Calculate the expectation value of the position $\langle x\rangle_t$ and momentum $\langle p\rangle_t$. Show that they satisfy the equations of motion

$$\langle p\rangle_t = m\frac{\mathrm{d}\langle x\rangle_t}{\mathrm{d}t}, \qquad \frac{\mathrm{d}\langle p\rangle_t}{\mathrm{d}t} = m\frac{\mathrm{d}^2\langle x\rangle_t}{\mathrm{d}t^2} = 0.$$

(2 points)

d) Compute the expectation values $\langle p^2\rangle_t$ and $\langle x^2\rangle_t$ and verify the validity of the uncertainty relation. (3 points)

Useful integrals

$$\int \mathrm{d}x\, \mathrm{e}^{-ax^2}\mathrm{e}^{-iqx} = \sqrt{\frac{\pi}{a}}\mathrm{e}^{-q^2/4a} \qquad \text{for } \mathrm{Re}(a) > 0,$$

$$\int \mathrm{d}k k^2 \mathrm{e}^{-k^2/b} = \frac{b}{2}\sqrt{b\pi}, \qquad \text{for } \mathrm{Re}(b) > 0.$$

PROBLEM 5: Time-independent perturbation theory

It is a good approximation to consider the ammonia molecule NH_3 as a two state system. The three H nuclei are in the same plane, and the N molecule is at a fixed distance either above or below the plane of the H's. Each state is approximately a stationary state with some energy E_0. There is a small amplitude for transition from up to down. Thus the Hamiltonian is $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}'$, where

$$\mathcal{H}_0 = \begin{pmatrix} E_0 & 0 \\ 0 & E_0 \end{pmatrix} \quad \text{and} \quad \mathcal{H}' = \begin{pmatrix} 0 & -A \\ -A & 0 \end{pmatrix} \tag{1}$$

where $|A| \ll E_0$

a) Find the exact eigenvalues E_a and E_b of $\mathcal{H}$. (2 points)

The eigenvalue equations are

$$\mathcal{H}|\psi_a\rangle = E_a|\psi_a\rangle \quad \text{and} \quad \mathcal{H}|\psi_b\rangle = E_b|\psi_b\rangle\,. \tag{2}$$

Now suppose the molecule is in an electric field, which distinguishes the two states with energy E_0. The new Hamiltonian becomes $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}' + V$, where

$$V = \begin{pmatrix} \epsilon_1 & 0 \\ 0 & \epsilon_2 \end{pmatrix}. \tag{3}$$

b) Find the new exact eigenvalues E_1 and E_2 of new $\mathcal{H}$. (2 points)

c) Applying time-independent perturbation theory, find the lowest order ΔE for $|\epsilon_i| \ll |A|$. (3 points)

d) Apply time-independent perturbation theory and find the lowest order ΔE for $|\epsilon_i| \gg |A|$. (3 points)

Hint: It is convenient to choose different unperturbed states in parts (c) and (d).

PROBLEM 6: Clebsh-Gordan coefficients

Consider two particles, one with spin $s_1 = \frac{1}{2}$ and a second with spin $s_2 = 1$.

a) If $\mathbf{S} = \mathbf{S}_1 + \mathbf{S}_2$ is the total spin operator, what are the possible quantum numbers associated with $\mathbf{S}^2$ and S_z? (2 points)

b) Write down the total spin states $|s, m\rangle$ in terms of product states $|s_1, m_1\rangle|s_2, m_2\rangle$, where m, m_1 and m_2 are the magnetic quantum numbers associated with S_z, $S_{z,1}$ and $S_{z,2}$ respectively. (3 points)

c) Suppose particle 2 is now decomposed into two spin 1/2 particles, resulting in three distinguishable spin 1/2 particles (we label them particles 1, 2 and 3). Express the total spin states $|s, m\rangle$ in terms of product states $|s_1, m_1\rangle|s_2, m_2\rangle|s_3, m_3\rangle$ of the three spin 1/2 particles. (3 points)

d) The Hamiltonian of the three particles considered in part c is

$$\mathcal{H} = \alpha(\mathbf{S}_1 \cdot \mathbf{S}_2 + \mathbf{S}_1 \cdot \mathbf{S}_3 + \mathbf{S}_2 \cdot \mathbf{S}_3),$$

Calculate the eigenenergies of the system and their degeneracies. (2 points)

Hint:

$$S_\pm = S_x \pm iS_y$$

$$S_\pm|s, m\rangle = \hbar\sqrt{(s \mp m)(s \pm m + 1)}|s, m \pm 1\rangle$$