Quantum Mechanics Qualifying Exam

Spring 2022

January 19 (9:00 am - 12:00 pm)

1. An ensemble of identical three-state quantum systems is described by a density matrix

$$\rho = \frac{1}{10}\begin{pmatrix} x & -2 & 0 \\ -2 & 6 & a \\ 0 & a & x \end{pmatrix}$$

(a) What must be the value of x?

(b) Is it possible for ρ to represent a pure quantum ensemble? What value would a need to have?

(c) Calculate the determinant of ρ and obtain from it the condition for a which makes ρ an acceptable density matrix. Show that $\det(\rho) < 0$ for the value of a you obtained in part (b). What does that mean? Is ρ with this value of a an acceptable density matrix (explain)?

2. An electron lives in the $d_{x^2-y^2}$ orbital of a certain atom. Its wavefunction has the form:

$$\psi(\mathbf{r}) = f(r)\,\frac{x^2-y^2}{r^2}$$

where $r = \sqrt{x^2+y^2+z^2}$ is the electron's distance from the nucleus.

(a) If one measures the square of the orbital angular momentum, what measurement outcomes are possible?

(b) If one measures the z-projection of the orbital angular momentum, what measurement outcomes are possible?

(c) What are the probabilities of all measurement outcomes you reported in the parts (a) and (b)?

(d) What is the smallest atomic number of an element that can hold a $d_{x^2-y^2}$ electron in its ground state?

3. A spinful particle is placed in magnetic field $\mathbf{B}$ and its Hamiltonian is $\hat{H} = -\mu\mathbf{B}\hat{\mathbf{S}}$, where $\hat{\mathbf{S}}$ is the vector of spin operators $\hat{S}_x, \hat{S}_y, \hat{S}_z$.

(a) Derive the equation of motion for the spin operator $\hat{\mathbf{S}}(t)$ in the Heisenberg picture. Start from the generic Heisenberg equation and obtain the time derivatives for all components of $\hat{\mathbf{S}}$ expressed in terms of the components of $\hat{\mathbf{S}}$ and $\mathbf{B}$.

(b) Suppose the particle has spin S, i.e. the measurement of $\hat{S}^2$ on it would yield $\hbar^2 S(S+1)$. If a measurement at time $t=0$ discovered that the particle's spin was pointed in the z-direction, and the magnetic field points along the x-direction, how much time δt needs to pass until the measurement of

S_y would yield $+\hbar S$ with certainty? At this time $t = \delta t$, does the spin point in the y-direction with absolute certainty (explain)?

(c) If $S = \frac{1}{2}$ in the scenario from part (b), what is the probability $P_z(t)$ that a measurement of S_z at time t would yield $+\frac{\hbar}{2}$?

4. A particle of mass m and charge e is trapped in a one-dimensional harmonic oscillator with potential $V(x) = \frac{1}{2}m\omega^2 x^2$. The particle is initially in the ground state, but suddenly, at some instant of time, a uniform electric field of strength $\mathcal{E}$ is turned on, adding $\delta V = -e\mathcal{E}x$ to the particle's potential energy.

(a) What energy and position expectation value $\langle x \rangle$ would the particle have in the ground state of the new potential? [Hint: find a way to express the new potential as another harmonic oscillator]

(b) What is the probability that the particle would be detected in the ground state of the new potential just after the electric is turned on? Does this probability change over time (explain)? [Hint: write the ground state wavefunctions for the old and new potentials, and use the postulate of quantum measurement; requres solving a Gaussian integral using the "square completion" approach]

(c) If the harmonic potential is suddenly turned off at $t = 0$ but the electric field is kept, how does the particle's expected position $\langle x \rangle$ change over time? Calculate $\langle x(t) \rangle$.

(d) If, instead, both the harmonic potential and electric field are turned off at $t = 0$, making the particle free, how does its wavefunction evolve over time? Derive a closed form of the normalized wavefunction $\psi(x,t)$. [Hint: this is the most difficult part]

Useful formulas:

- Gaussian integral:

$$\int_{-\infty}^{\infty} dx\, e^{-\alpha x^2} = \sqrt{\frac{\pi}{\alpha}}$$

- Harmonic oscillator and its ground state wavefunction:

$$H = \frac{\hat{p}^2}{2m} + \frac{m\omega^2 x^2}{2} \quad , \quad \psi_0(x) = \left(\frac{1}{\pi\xi^2}\right)^{\frac{1}{4}} e^{-x^2/2\xi^2} \quad ; \quad \xi = \sqrt{\frac{\hbar}{m\omega}}$$

- Pauli matrices:

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

$$e^{i\boldsymbol{\sigma}\hat{\mathbf{n}}\theta} = \cos\theta + i(\boldsymbol{\sigma}\hat{\mathbf{n}})\sin\theta$$

- Spherical harmonics:

$$Y_0^0 = \sqrt{\frac{1}{4\pi}}$$

$$Y_1^0 = \sqrt{\frac{3}{4\pi}}\cos\theta \quad , \quad Y_1^{\pm 1} = \mp\sqrt{\frac{3}{8\pi}}\sin\theta\, e^{\pm i\phi}$$

$$Y_2^0 = \sqrt{\frac{5}{16\pi}}(3\cos^2\theta - 1) \quad , \quad Y_2^{\pm 1} = \mp\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta\, e^{\pm i\phi} \quad , \quad Y_2^{\pm 2} = \sqrt{\frac{15}{32\pi}}\sin^2\theta\, e^{\pm 2i\phi}$$