Quantum Mechanics Qualifying Exam

Fall 2024: August 21, 9:00 am - 12:00 pm

Every problem is worth 25 points.

1. (a) A particle is set in free rightward motion with energy $E > U_0 > 0$ and approaches a step potential

$$U(x) = \begin{cases} 0 & , \quad x < 0 \\ U_0 & , \quad x > 0 \end{cases}$$

from the left side. Derive the probability $T(E)$ that the particle will cross the step and be detected far away from it on its right side. What is this probability if $E < U_0$?

(b) A thermal ensemble of particles is prepared at temperature T. What density matrix describes this ensemble if the particle dynamics is governed by the Hamiltonian H?

(c) What density matrix describes the quantum-statistical probability distribution of the particles which originated in the thermal ensemble prepared far to the left of the step, and were detected far to the right of the step? Do not include in the ensemble the particles which reflected back from the step. It is sufficient to specify the eigenvalues of this density matrix. Is the ensemble of detected particles canonically thermal?

2. A valence electron of some atom is prepared in the state whose wavefunction is

$$\psi(x, y, z) = f(r)(x - y + iz)$$

at time $t = 0$. The "radial" function $f(r)$ is determined by the spherically symmetric electrostatic potential inside the atom, where r is the distance from the nucleus at the origin. A uniform external magnetic field $\mathbf{B} = B\hat{\mathbf{z}}$ affects the electron's motion through the Zeeman coupling to its angular momentum, as expressed in the Hamiltonian

$$H = -\gamma \mathbf{L}\mathbf{B} = -\gamma B L_z$$

(a) What is the probability that the electron will be detected at $t = 0$ in a state with zero projection of the angular momentum on the z-axis?

(b) Where in space is it not possible to detect the electron at $t = 0$? Specify the coordinates $\mathbf{r} = (x, y, z)$ of such points, assuming $f(r) \neq 0$.

(c) What is the answer to part (b) at an arbitrary time $t > 0$? A qualitatively correct and justified guess will be accepted for full credit, while a correct detailed derivation will earn extra credit.

3. A molecule consists of three different atoms, labeled by $n = 1, 2, 3$. An electron can be localized on any of these atoms with zero energy, except for one atom where the energy is ϵ. The electron can also tunnel from an atom to any other atom with the same probability. The Hamiltonian can be constructed in the position representation as (with t being a "tunneling" energy coefficient):

$$H = \begin{pmatrix} \epsilon & t & t \\ t & 0 & t \\ t & t & 0 \end{pmatrix} = t \begin{pmatrix} \frac{\epsilon}{t} & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$$

(a) Find the energy spectrum of electron's stationary states.

(b) One of the Hamiltonian eigenvalues is $E = -t$. Find the vector representation of the stationary state $|-t\rangle$ that has this energy.

(c) The molecule is symmetric under the exchange of atoms 2 and 3, which impart the same zero potential energy on the electron. Construct the unitary operator M which carries out this mirror symmetry transformation, in the same representation as H. Does the stationary state $|-t\rangle$ possess the mirror symmetry (check if the mirror transformation changes it)? If yes, what is its parity under a mirror transformation?

4. An artificially engineered quantum system is governed by the one-dimensional Hamiltonian

$$H = \hbar\omega \cos\left[\frac{\phi}{\hbar\omega}\left(\frac{p^2}{2m} + \frac{m\omega^2 x^2}{2}\right)\right]$$

where p and x are the usual momentum and position operators respectivelly. Note that the cosine of an operator can always be defined by its Taylor expansion, which contains only the well-defined operator powers.

(a) Determine the entire energy spectrum.

(b) For which values of the dimensionless parameter ϕ does the entire spectrum reduce to a finite set of energy levels with infinite degeneracy? How many of such distinct energy levels are there for the given ϕ?

(c) What kind of spectrum is obtained if ϕ does not have any value identified in part (b)? On one hand, the spectrum is discrete because energy levels are enumerated by an integer-valued quantum number n. But, on the other hand, infinitely many energy levels (for all n) must fit in a finite energy "band", $-\hbar\omega \le E_n \le \hbar\omega$. Do the energy levels form a continuous band, given that they do not collapse on a finite number of distinct values? If yes, are the wavefunctions extended states?

Useful formulas:

- Spherical harmonics:

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

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

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

- Probability current density in one dimension:

$$j = -\frac{i\hbar}{2m}\left(\psi^*\frac{d\psi}{dx} - \psi\frac{d\psi^*}{dx}\right)$$