INTERNATIONAL INSTITUTE OF INFORMATION TECHNOLOGY HYDERABAD

QUANTUM MECHANICS

Monsoon 2022 – CND Core – Credit 4

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Date: NOVEMBER 19, 2022

Time: 03 H 00 M

End Examination

Total Marks: 100

Instructions:

- Keep your answers **to the point**. You may skip 'trivial' steps. However, unless the logic is clear, you will **not** get any credit for a problem.
- Illegible answers will **not** be graded.
- **No** 'benefit of doubt' because of bad notation/illegible hand-writing etc.

Q 1. Consider a finite square well,

$$V(x) = \begin{cases} -V_0 & \text{for } -a < x < a \quad (V_0 > 0) \\ 0 & \text{otherwise,} \end{cases}$$

with a particle of energy $E > 0$ (scattering state).

(a) Show that the probability of the particle reflecting back is nonzero in general.

(b) What happens if $E \gg V_0$ or $E \to 0$? Show that there are some energies for perfect transmission (transmission resonance, this is why you get a very large transmission when you scatter low-energy electrons through noble-gas atoms).

(c) We say that *the absolute value of potential does not matter, only the difference matters. Hence, if we add a constant to the overall potential, nothing changes.* Is this true in Quantum Mechanics? If so, how do we see that? If not, why not?

[3+3+4=10] CO: 1,4,5

Q 2. (a) Show with the momentum-space wave function $\Phi(p,t)$ that

$$\langle x \rangle = \int \Phi^* \left(-\frac{\hbar}{i} \frac{\partial}{\partial p} \right) \Phi \, dp.$$

(b) Prove the Virial theorem:

$$\frac{d}{dt} \langle xp \rangle = 2 \langle T \rangle - \left\langle x \frac{dV}{dx} \right\rangle,$$

where T is the kinetic energy.

(c) Consider a periodic potential, i.e., $V(x+\lambda) = V(x)$. Show that the wave function at $(x_0+\lambda)$ is proportional to $\psi(x_0)$ up to a constant (i.e., x-independent) phase.

(d) Explain how one gets dynamic solutions out of the stationary states for the time-independent potential.

(e) Show that for a simple harmonic oscillator $\langle \hat{V} \rangle = \langle \hat{T} \rangle$.

[2+3+3+2+5=15] CO: 1,3,4,5

Q 3. A spinning electron constitutes a magnetic dipole. Its dipole moment is proportional to the spin,

$$\vec{\mu} = \gamma \vec{S}$$

where γ is the gyromagnetic ratio. If you put it in a magnetic field $\vec{B}$, it feels a torque. The energy associated with the torque is $-\vec{\mu} \cdot \vec{B}$.

(a) If the magnetic field is constant $\vec{B} = B_0 \hat{z}$, then show that $< \vec{S} >$ gets titled and it precesses about the field with a constant frequency.

(b) If $\vec{B} = B_0 \cos(\omega t) \hat{z}$ (where ω is a constant) and the electron starts out in the spin-up state in the x direction, i.e.,

$$\chi(0) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix},$$

then obtain $\chi(t)$ by solving the time dependent Schrödinger equation

$$i\hbar \frac{\partial \chi}{\partial t} = \mathbf{H} \chi,$$

where $\mathbf{H}$ is the Hamiltonian matrix.

[7+8=15] CO: 2,3,4

Q 4. (a) Let, for a system of interest $\{|a_i\rangle\}$ be the set of eigenstates of an Hermitian operator A. Show that

(i) the matrix $A_{ij} = \langle a_i|A|a_j\rangle$ is diagonal,

(ii) the matrix $B_{ij} = \langle a_i|B|a_j\rangle$ is also diagonal where A and B are compatible observables.

(iii) the transformation from the basis $\{|a_i\rangle\}$ to another basis $\{|c_i\rangle\}$ is unitary, where $\{|c_i\rangle\}$ are the eigenstates of another Hermitian operator C incompatible with A or B.

(b) In the case of perturbation theory with degenerate states, why does one first look for some operator that commutes with the perturbed Hamiltonian?

(c) If the lowest-order relativistic correction to the Hamiltonian is given as

$$H' = -\frac{p^4}{8m^3c^2},$$

find the lowest-order relativistic correction to the energy levels of the one-dimensional harmonic oscillator.

[(1+2+2)+3+7=15] **CO:** 1,2,4,5

Q 5. Use a Gaussian trial function, $\psi(x) = \left(\frac{2b}{\pi}\right)^{1/4} e^{-bx^2}$ to obtain the lowest upper bound on the ground state energy of

(a) the linear potential: $V(x) = \alpha|x|$,

(b) the quartic potential: $V(x) = \alpha x^4$.

[5+5=10] **CO:** 3,4

Q 6. (a) Show that the x, y and z components of the angular momentum operator $(\hat{L}_x, \hat{L}_y, \hat{L}_z)$ are mutually incompatible but all of them commute with $\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$ (it is sufficient to show that $\hat{L}^2$ commutes with any one component, say $\hat{L}_z$, the rest can be argued similarly).

(b) Since $\hat{L}^2$ and $\hat{L}_z$ commute, lets denote their common eigenstates as $|\lambda,\mu\rangle$ where

$$\hat{L}^2|\lambda,\mu\rangle = \lambda|\lambda,\mu\rangle \quad \text{and} \quad \hat{L}_z|\lambda,\mu\rangle = \mu|\lambda,\mu\rangle.$$

Now, with the following operators

$$\hat{L}_\pm = \hat{L}_x \pm i\hat{L}_y$$

show that

$$[\hat{L}_z, \hat{L}_\pm] = \pm\hbar\hat{L}_\pm \quad ; \quad [\hat{L}^2, \hat{L}_\pm] = 0 \quad ; \quad \hat{L}^2 = \hat{L}_\pm\hat{L}_\mp + \hat{L}_z^2 \mp \hbar\hat{L}_z \quad \text{and}$$

(c) the operators $\hat{L}_\pm$ take one eigenstate to another eigenstate as:

$$\hat{L}_\pm|\lambda,\mu\rangle \propto |\lambda,\mu\pm\hbar\rangle,$$

i.e., they act like ladder operators. In other words, show that

$$\begin{aligned} \hat{L}^2\left(\hat{L}_\pm|\lambda,\mu\rangle\right) &= \lambda\left(\hat{L}_\pm|\lambda,\mu\rangle\right), \\ \hat{L}_z\left(\hat{L}_\pm|\lambda,\mu\rangle\right) &= (\mu\pm\hbar)\left(\hat{L}_\pm|\lambda,\mu\rangle\right). \end{aligned}$$

(d) Now, there will be a μ_{max} and a μ_{min}, i.e., if we start with some $|\lambda,\mu\rangle$ and keep on applying $\hat{L}_+$ on it, the process will terminate when we apply $\hat{L}_+$ on $|\lambda,\mu_{max}\rangle$ and, similarly, $\hat{L}_-|\lambda,\mu_{min}\rangle = 0$. Show that λ for the μ_{max} state will be given as

$$\lambda = \mu_{max}(\mu_{max}+\hbar) \quad \text{and} \quad \mu_{min} = -\mu_{max}.$$

(e) Finally show

$$\hat{L}_\pm|\lambda,\mu\rangle = \sqrt{\mu_{max}(\mu_{max}+\hbar) - \mu(\mu\pm\hbar)}\,|\lambda,\mu\pm\hbar\rangle.$$

[5+4+(2+2)+(2+2)+3=20] **CO:** 1,2,3

Q 7. Consider a box of volume V containing free electron gas (assume the total number of atoms to be N with each one contributing q electrons). The normalized wave functions are given as

$$\psi_{n_x,n_y,n_z} = \sqrt{\frac{8}{V}}\sin\left(\frac{n_x\pi}{l_x}x\right)\sin\left(\frac{n_y\pi}{l_y}y\right)\sin\left(\frac{n_z\pi}{l_z}z\right)$$

where $V = l_x l_y l_z$. The allowed energies are

$$E_{n_x,n_y,n_z} = \frac{\hbar^2k^2}{2m} = \frac{\hbar^2}{2m}(k_x^2+k_y^2+k_z^2)$$

where the wave vector $\vec{k} = (k_x, k_y, k_z)$ with $k_i = n_i^2/l_i^2$.

(a) Show that the Fermi energy is $E_F = \frac{\hbar^2}{2m}(3\rho\pi^2)^{2/3}$ where ρ is the free electron density. How is it related to the chemical potential?

(b) The total energy $E_{tot} \propto V^{-2/3}$. Find the proportionality constant and the degeneracy pressure.

(c) Covalent bonding between two electrons requires the two to be in the singlet state. Explain.

[4+6+5=15] CO: 1,4,5