Quantum Mechanics

August 19, 2021

Work 4 (and only 4) of the 5 problems. Please put each problem solution on a separate sheet of paper and your name on each sheet.

Problem 1

A point particle of mass m and charge q is subjected simultaneously to a magnetic and an electric field: $\vec{B} = B_0\hat{z}$ and $\vec{E} = E_0\hat{x}$ (where B_0 and E_0 are the strength of the magnetic and electric field respectively, and $\hat{x}$ is the unit vector in the Cartesian x-direction).

a.) Compute the **complete** energy spectrum and comment on the occurrence of degeneracies.

b.) Evaluate the expectation value of the velocity $\vec{v}$ in a state of zero momentum. What is its direction?

Problem 2

Consider a charged particle in a two-dimensional isotropic harmonic oscillator with an electric field that rotates as a function of time. The Hamiltonian is

$$\hat{\mathcal{H}}(t) = \hat{\mathcal{H}}_0 + \hat{\mathcal{H}}_1(t) \tag{1}$$

with

$$\hat{\mathcal{H}}_0 = \frac{\hat{\vec{p}}^2}{2m} + \frac{1}{2}m\omega^2\hat{\vec{r}}^2 = \frac{\hat{p}_x^2 + \hat{p}_y^2}{2m} + \frac{1}{2}m\omega^2(\hat{x}^2 + \hat{y}^2)\,, \tag{2a}$$

$$\hat{\mathcal{H}}_1(t) = -q\vec{\mathcal{E}}(t)\cdot\hat{\vec{r}} = -q\mathcal{E}\left(\cos\Omega t\,\hat{x} + \sin\Omega t\,\hat{y}\right)\,, \tag{2b}$$

where m and q are the mass and charge of the particle, $\mathcal{E}$ is the constant magnitude of the electric field, and ω and Ω are the frequencies of the oscillator and the rotating electric field, respectively.

a.) *(1 pt.)* Write out explicitly the time-dependent Schrödinger equation for the time dependence of an arbitrary quantum state $|\psi\rangle$ under the action of the Hamiltonian $\hat{\mathcal{H}}$ from Eq. (1).

b.) *(1 pt.)* Let us define a transformed quantum state $|\psi_R\rangle$ which is obtained from the original quantum state $|\psi\rangle$ by

$$|\psi_R(t)\rangle \equiv \exp\left[-\frac{i}{\hbar}\hat{L}_z\,\Omega t\right]\,|\psi(t)\rangle \tag{3}$$

with $\hat{L}_z$ the angular momentum operator. Describe briefly in words what the transformation (3) does to the quantum state $|\psi\rangle$.

c.) *(2 pts.)* Insert the transformation (3) into the time-dependent Schrödinger equation to obtain an equation for the time dependence of $|\psi_R\rangle$. Show that this equation again takes the form of the time-dependent Schrödinger equation but with a transformed Hamiltonian $\hat{\mathcal{H}}_R$ and express $\hat{\mathcal{H}}_R$ in terms of $\hat{\mathcal{H}}$. *(You do not need to fully evaluate $\hat{\mathcal{H}}_R$ yet, just find how it relates to $\hat{\mathcal{H}}$.)*

d.) *(3 pts.)* Explicitly evaluate $\hat{\mathcal{H}}_R$ and show that, in terms of the transformed coordinate operators

$$\begin{bmatrix}\hat{x}_R\\ \hat{y}_R\end{bmatrix} \equiv \begin{bmatrix}\cos\Omega t & \sin\Omega t\\ -\sin\Omega t & \cos\Omega t\end{bmatrix}\begin{bmatrix}\hat{x}\\ \hat{y}\end{bmatrix}\,, \tag{4}$$

the transformed Hamiltonian $\hat{\mathcal{H}}_R$ is time-independent. *(Hint: Recall that $\hat{L}_z$ commutes with any scalar operator, and keep in mind the physical meaning of the transformation (3).)*

e.) *(1.5 pts.)* Compute the eigenvalues of $\hat{\mathcal{H}}_R$ and then transform back to find the eigenvalues of the original Hamiltonian $\hat{\mathcal{H}}$ from Eq. (1). *(Hint: Complete the square and use the known eigenvalues of the usual harmonic oscillator.)*

f.) *(1.5 pts.)* Given that the ground state wave function of the 2D harmonic oscillator (2a) is the Gaussian wave packet

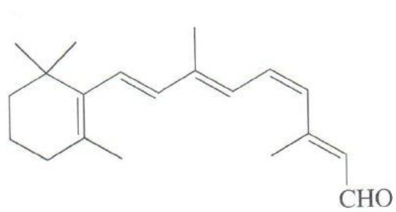
$$\psi_{0,HO}(x,y) = \sqrt{\frac{m\omega}{\pi\hbar}} \exp\left[-\frac{m\omega}{2\hbar}(x^2+y^2)\right] , \tag{5}$$

find the ground state of the original Hamiltonian $\hat{\mathcal{H}}$ from Eq. (1). What is the wave packet doing as a function of time?

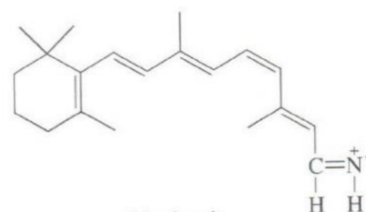
Problem 3

a.) Refer to the structural formulas depicted below. Using the free-electron molecular orbital (particle-in-a-box) model for a conjugated system, explain why the absorption maximum of Rhodopsin is at a higher wavelength than that of 11-cis retinal.

b.) Using the free-electron molecular orbital model, calculate the wavelength of maximum absorbance for 11-cis retinal and for rhodopsin, taking the average value of $1.39 \cdot 10^{-10}$ m and adding one bond length to each end of the conjugated system of bonds. Remember to count the pi-electrons and assign two to each space orbital in accordance with the Aufbau principle.



11-*cis*-Retinal



Rhodopsin

Problem 4

Using variational methods and a suitable test wavefunction of your choice, estimate the ground state energy of a particle of mass m in a potential $V(x) = Ax^4$, where A is some constant $(A > 0)$.

Problem 5

a.) A deuterium atom (D) is like the hydrogen atom (H), except that the nucleus consists of a proton and a neutron, i.e. the nucleus in D has about twice the mass as in H. Which of the following is true for the ground state binding energy for the e^- in D: The energy required to excite D from the ground state to the 1^{st} excited state is (2 points)

i.) about half that in H
ii.) slightly smaller than in H
iii.) the same as in H
iv.) slightly bigger than in H
v.) about twice that in H

Explain your answer:

b.) A particle of mass m is in the ground state of the harmonic oscillator in one dimension. The classical angular frequency is ω. What is the expectation value $\langle p^2 \rangle$ for this particle? Explain your answer! Hint: you may use that for the harmonic oscillator the expectation value of the kinetic energy equals the expectation value of the potential energy. (2 points)

c.) Consider a particle of mass m in a harmonic oscillator potential in two dimensions, $V(x, y) = \frac{k}{2}(x^2 + y^2)$. (4 points)

i.) What is the energy of the ground state? And what is its degeneracy?

ii.) What is the energy of the first excited state and what is its degeneracy?

iii.) Now suppose an additional potential energy $\Delta V(x, y) = V_0 \delta(x)$ is added, with V_0 being a positive constant. Qualitatively, what happens to these energy levels? Do they go up or down or stay the same? Answer this question separately for each of the energy levels that you identified above.

d.) What is the ground state energy for a system of two identical spin $\frac{1}{2}$ particles of mass m in three dimensions, both with spin $|\uparrow\rangle$, when a potential $V(\vec{r}_1 - \vec{r}_2) = \frac{k}{2}(\vec{r}_1 - \vec{r}_2)^2$ acts between them? (2 points)