Quantum Mechanics 2026 HW7

Due 11/18 in Class

November 12, 2026

Problem 1. Hydrogen atom wavefunction

1) Write down the expression of $\psi_{n_r,l,m}(r,\theta,\phi)$, where n_r is the radial quantum number, l and m are the quantum numbers of angular momentum quantum (OAM) and the z-component of OAM, respectively. Write down the relation of the energy E and the quantum numbers.

(You do not need to derive them again. I do want you to write down the expression of the hyper-geometric polynomials. You do not need to write down the normalization constant.)

2) Write down the *normalized* expressions of $\psi_{n,l,m}(r,\theta,\phi)$ with $n = n_r + l + 1$ for $n = 1$, 2, 3. In fact, they are the wavefunctions of $1s$; $2s$, $2p$; $3s$, $3p$, and $3d$ orbitals of the hydrogen atom. Sketch the radial part of the wavefunction $R_{n,l}(r)$. Please notice in which states there appear cusps and argue why the cusps appear?

Problem 2. Gaussian orbital approximation

By solving this problem, you will have some basic senses of the Nobel prize of Chemistry in 1998 by John Pople.

1) Consider the $1s$ orbital of hydrogen atom $\psi_{1s}(\mathbf{r})$. Approximate the $1s$ orbital with the Gaussian orbital $\psi^G_{1s}(\mathbf{r}) = Ne^{-\frac{r^2}{\lambda^2}}$, where N is the normalization factor. Calculate $Err(\lambda) = \int d\mathbf{r}|\psi_{1s}(\mathbf{r}) - \psi^G_{1s}(\mathbf{r})|^2$, and minimize it with respect to λ.

2) Use the Gaussian orbital approximation to calculate the overlap integral between two $1s$-orbital of two hydrogen atoms, i.e., $\int d^3\mathbf{r}\psi^*_{1s}(\mathbf{r})\psi_{1s}(\mathbf{r} - l_0\hat{z})$

In terms of the chemistry jargon, approximately this is proportional to the σ-bonding strength.

Problem 3. 2D hydrogen atom

Read my lecture notes. Solve the hydrogen atom problem in 2D, i.e.,

$$H = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{r} \tag{1}$$

. You do not need to normalize the wavefunction. Compare the eigen-energies and the energy level degeneracies between the 2D and the 3D cases.

Problem 4. Schwinger boson representation of angular momentum

Consider a 2D harmonic oscillator $H = \hbar\omega(a_1^\dagger a_1 + a_2^\dagger a_2)$ exhibiting the SU(2) symmetry. Define $a = (a_1, a_2)^T$ and $a^\dagger = (a_1^\dagger, a_2^\dagger)$. Define $J_\mu = \frac{1}{2} a_\alpha^\dagger \sigma_{\alpha\beta}^\mu a_\beta$ where σ^μ are Pauli matrices with $\mu = x, y, z$.

1) Prove that $[J_\mu, J_\nu] = i\epsilon_{\mu\nu\lambda} J_z$.

2) Define $2J = a^\dagger a$, then $J_x^2 + J_y^2 + J_z^2 = J(J+1)$.

3) Define $|jm\rangle = \frac{(a_1^\dagger)^{j+m}}{\sqrt{(j+m)!}} \frac{(a_2^\dagger)^{j-m}}{\sqrt{(j-m)!}} |00\rangle$. Then prove $J_z|jm\rangle = m|jm\rangle$, and $J_\pm|jm\rangle = \sqrt{(j \mp m)(j \pm m + 1)}|jm \pm 1\rangle$.

Problem 5. CG coefficients

Organize two sets of angular momentum $J_1 = J_2 = 1$ states $|1m_1\rangle$ and $|1m_2\rangle$ into the total angular momentum $J = J_1 + J2$ and J_z. Please figure out the CG coefficients for the expansion of

$$|JJ_z\rangle = \sum_{m_1, m_2} \langle JJ_z | lm_1 lm_2\rangle |1m_1\rangle |1m_2\rangle. \tag{2}$$

Problem 6. SO coupling

Inside atoms, besides the Coulomb interaction there exists spin-orbit (SO) coupling. Below we consider a simplified version of SO coupling

$$H_{so} = \omega \sigma \cdot \mathbf{L}, \tag{3}$$

and we will solve its eigenvalues and eigenstates. We consider the spherical harmonic function $Y_{lm}(\theta, \phi)$ with the quantum number l and couple it with electron's spin-$\frac{1}{2}$. We start from the basis $|lm; ssz\rangle$ defined as

$$|lm\rangle \otimes |\tfrac{1}{2}\tfrac{1}{2}\rangle = \begin{pmatrix} Y_{lm}(\theta, \phi) \\ 0 \end{pmatrix}, \tag{4}$$

$$|lm\rangle \otimes |\tfrac{1}{2} - \tfrac{1}{2}\rangle = \begin{pmatrix} 0 \\ Y_{lm}(\theta, \phi) \end{pmatrix}. \tag{5}$$

1) There are two sets of different eigenvalues of H_{so} denoted as E_+ and E_-. For the $E_\pm$-sectors, the normalized eigenstates are denoted as $Y_{j_+, j_z}(\theta, \phi)$ and $Y_{j_-, j_z}(\theta, \phi)$, respectively. $Y_{j_\pm, j_z}(\theta, \phi)$ are eigenstates of total angular momentum $\mathbf{J}^2$ and J_z with eigenvalue $j_\pm(j_\pm + 1)$ and j_z, respectively. These are called sectors with positive and negative helicities, respectively.

What are the values of $j_\pm$? What are the values of E_+ and E_-?

(Hint: you may use the operator identity $\sigma \cdot \mathbf{L} = \mathbf{J}^2 - \mathbf{L}^2 - \mathbf{S}^2$, where $\mathbf{S} = \frac{\hbar}{2}\sigma$ and $\mathbf{J} = \mathbf{L} + \mathbf{S}$. Please note that $\mathbf{L}$, $\mathbf{S}$, and $\mathbf{J}$ are all operators.)

2) Consider the case that $l = 1$. Express $Y_{j_\pm, j_z}$ as

$$Y_{j_\pm, j_z}(\theta, \phi) = \begin{pmatrix} a_{j_\pm, j_z} Y_{lm}(\theta, \phi) \\ b_{j_\pm, j_z} Y_{lm+1}(\theta, \phi). \end{pmatrix}. \tag{6}$$

Derive the expressions $a_{j_\pm, j_z}$ and $b_{j_\pm, j_z}$.