Quantum Mechanics 2025 HW7

Due 11/04 in Class

October 25, 2025

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) Consider the $2p_z$ orbital of a hydrogen atom. Approximate it with the Gaussian orbital $\psi^G_{2p_z}(\mathbf{r}) = Nze^{-\frac{r^2}{\lambda^2}}$, where N is the normalization factor. Use the similar method to optimize the value of λ.

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

4) Use the Gaussian orbital approximation to calculate the following two overlap integrals between two $2p_z$ hydrogen atoms a) $\int d^3\mathbf{r}\psi^*_{2p_z}(\mathbf{r})\psi_{2p_z}(\mathbf{r} - l_0\hat{z})$ and b) $\int d^3\mathbf{r}\psi^*_{2p_z}(\mathbf{r})\psi_{2p_z}(\mathbf{r} - l_0\hat{x})$.

In terms of the chemistry jargon, approximately the former is proportional to the σ-bonding strength, and the latter is proportional to the π-bonding. Which one is stronger?

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. Edge spectrum of the edge state of QHE

Read my lecture notes, and derive the edge state spectrum of a QHE system for a system with the disk geometry.

Problem 5. 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 6. 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

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