

Three dimensional problems

Assignment 3
Quantum Mechanics 1, 2008

These assignments will be graded, and the grades will count towards the final consolidated performance in the course. The assignment is due on October 27. Every day's delay after that will cause a 10% loss in marks. Use Mathematica wherever necessary; mention that in your answer sheet and submit the notebook also.

- Construct the direct product of two $l = 1$ representations of angular momentum.
 - Write down the matrices for \mathbf{L} and L^2 in the direct product basis.
 - What unitary transformation converts this to the direct sum of $l = 0, 1$ and 2 ?
 - Using your construction write down all the non-vanishing Clebsch-Gordan coefficients in this case.
 - Find the symmetries of the states of different total l under interchange of the two individual spins.
- For the isotropic harmonic oscillator in three dimensions, the eigenstates of the Hamiltonian for the $E = 7\hbar\omega/2$ level can be written either in the $|n_x, n_y, n_z\rangle$ basis or in $|n, l, m\rangle$. Find the unitary transformation between them.
- Expand $\exp(i\mathbf{k} \cdot \mathbf{r})$ in terms of spherical harmonics. Show that the expansion coefficients are spherical Bessel functions.
- For the rotationally symmetric potentials $V(r) = \pm V_0$ (for $r < a$) and zero otherwise, find the energy levels and eigenstates of the Hamiltonian. Are there analogues of the universal features found in the corresponding one-dimensional problem? If yes, then are there any quantitative differences in the universal exponents?
- Consider the H_2^+ ion. Take the line joining the two nuclei to be the z axis, and let the distance between them be a fixed quantity r_0 . The Hamiltonian for the electron is $H_e = p^2/2m - e^2/r_1 - e^2/r_2$, where r_i is the distance between the i -th nucleus and the electron. The symmetries of H_e are those of rotations around the z -axis: called $SO(2)$, and interchange of the two nuclei (corresponding to change of sign of z). The total Hamiltonian is $H = H_e + E_{pp}$, where $E_{pp} = e^2/r_0^2$ is the Coulomb energy of the two nuclei, neglecting the kinetic energy of the nuclei. Our approximation amounts to treating E_{pp} as a c-number.
 - Choose as basis states for the molecule the hydrogen atom states $|1; nlm\rangle$ and $|2; nlm\rangle$ centered at each of the nuclei. Any two states, $|\alpha\rangle$ and $|\beta\rangle$, are said to mix with each other if $\langle\alpha|H_e|\beta\rangle \neq 0$. Which of the basis states can mix with each other?
 - Is there a simplification if one starts from the basis states obtained by solving the Hydrogen atom problem in parabolic coordinates?
 - Choose a truncated Hamiltonian matrix with basis states chosen to be the two $n = 1$ states (this gives a 2×2 matrix). Diagonalize H_e to find the ground state. Plot the total energy of the ground state (i.e., the expectation value of H) as a function of r_0/a_0 (a_0 is the Bohr radius of Hydrogen). What is the minimum binding energy? What is the equilibrium distance between the nuclei? What is the level spacing for vibrational excitations?
 - Choose a truncated Hamiltonian matrix with basis states chosen to be $n = 1$ and 2 (this gives a 10×10 matrix). Block diagonalize this truncated Hamiltonian according to the symmetries of the problem. Enumerate the states which mix with each other.
 - The ground state of the system is expected to be scalar under the symmetries of H_e . In the 10×10 matrix above, find the 3×3 block which contributes to the ground state. Diagonalize this to find the expectation of H in the ground state. Plot this as a function of r_0/a_0 . What is the minimum binding energy? What is the equilibrium distance between the nuclei? What is the level spacing for vibrational excitations?
 - (This part is for extra credit only) Write a Mathematica program which will repeat this process for any n , i.e., given the principal quantum number n , it will set up corresponding truncated Hamiltonian for H_2^+ , find the equilibrium distance between nuclei, find the binding energy, and compute the level spacings for vibrational excitations. Using this program check whether there is a sensible limit to these quantities as n increases.