PHY403 Atomic and Molecular Physics Aug-Dec 2019: Tutorial 3

Dr. Kavita Dorai, Department of Physics, IISERM, kavita@iisermohali.ac.in

1. Use the variational method and a Gaussian trial wave function $\psi(x) = Ae^{-bx^2}$ to find the lowest upperbound on the ground state energy of the (a) linear potential $V(x) = \alpha|x|$ and the (b) quartic potential $V(x) = \alpha x^4$.

2. A corollary to the variational principle states that if $\langle\psi|\psi_g\rangle = 0$ then $\langle H\rangle \geq E_f$, where E_f is the energy of the first excited state and ψ_g is the exact ground state eigenfunction. So if one can find a trial function which is orthogonal to the exact ground state, then one can get an upper bound on the first excited state. If the potential $V(x)$ is an even function of x, the ground state is also even and any odd trial wavefunction will satisfy the corollary. Find the best bound on the first excited state of the one dimensional harmonic oscillator using trial wave function $\psi(x) = Axe^{-bx^2}$.

3. Apply the variational techniques used to find the ground state of helium, to find the best upper bound on E_g for the case of H^- and Li^+ ions. Each has two electrons like helium but with nuclear charges $Z = 1$ and $Z = 3$, respectively.

4. If the photon had a nonzero mass ($m_\gamma \neq 0$), the Coulomb potential will get replaced by a Yukawa potential

$$V(\mathbf{r}) = -\frac{e^2}{4\pi\epsilon_0}\frac{e^{-\mu r}}{r}$$

   where $\mu = m_\gamma c/\hbar$. Use any trial wave function of your choice and this potential and the variational method and find the binding energy of a hydrogen atom.

5. Let a quantum system have a Hamiltonian H_0 with only two orthogonal, normalized, nondegenerate eigenstates ψ_a (energy E_a) and ψ_b (energy E_b). Assume $E_a < E_b$. Turn on a perturbation H' with the following matrix elements:

$$\begin{aligned} \langle\psi_a|H'|\psi_a\rangle &= \langle\psi_b|H'|\psi_b\rangle = 0 \\ \langle\psi_a|H'|\psi_b\rangle &= \langle\psi_b|H'|\psi_a\rangle = h \end{aligned}$$

   Find the exact eigenvalues of the perturbed Hamiltonian and estimate the energies using second-order perturbation theory. Estimate the ground state energy of the perturbed system using the variational method, with a trial wave function of the form:

$$\psi = (\cos\phi)\psi_a + (\sin\phi)\psi_b$$

   where ϕ is an adjustable parameter.