Solutions to Assignment 2, UCSD Physics 130b

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1. Griffiths 5.1

Let us consider the quantities $\vec{r} = \vec{r_1} - \vec{r_2}$, $\vec{R} = \frac{m_1\vec{r_1}+m_2\vec{r_2}}{M} = \frac{\mu}{m_2}\vec{r_1} + \frac{\mu}{m_1}\vec{r_2}$, $M = m_1 + m_2$, $\mu = \frac{m_1 m_2}{M}$. Using these we see that,

$$\vec{R} = \frac{\mu}{m_2}\vec{r_1} + \frac{\mu}{m_1}(\vec{r_1} - \vec{r}) = \vec{r_1} - \frac{\mu}{m_1}\vec{r} \Rightarrow \vec{r_1} = \vec{R} + \frac{\mu}{m_1}\vec{r} \tag{1}$$

Similarly we find that,

$$\vec{r_2} = \vec{R} - \frac{\mu}{m_2}\vec{r} \tag{2}$$

To determine the gradient operators, we first define $\vec{r} = (\mathcal{X}, \mathcal{Y}, \mathcal{Z})$ and $\vec{R} = (X, Y, Z)$. Then we note that,

$$\frac{\partial}{\partial x_1}f(\vec{r}, \vec{R}) = \frac{\partial \mathcal{X}}{\partial x_1}\frac{\partial f}{\partial \mathcal{X}} + \frac{\partial X}{\partial x_1}\frac{\partial f}{\partial X} \tag{3}$$

Similarly for all other components of $\vec{r_1}$ and $\vec{r_2}$. Now, $\frac{\partial \mathcal{X}}{\partial x_1} = 1$ and $\frac{\partial \mathcal{X}}{\partial x_2} = -1$, as well as other permutations of this involving the y and z component. Also, we can see that $\frac{\partial X}{\partial x_1} = \frac{\mu}{m_1}$ and $\frac{\partial X}{\partial x_2} = \frac{\mu}{m_2}$. We can thus write,

$$\nabla_1 = (\frac{\partial}{\partial x_1}, \frac{\partial}{\partial y_1}, \frac{\partial}{\partial z_1}) = \nabla_r + \frac{\mu}{m_2}\nabla_R \tag{4}$$

Similarly,

$$\nabla_2 = (\frac{\partial}{\partial x_2}, \frac{\partial}{\partial y_2}, \frac{\partial}{\partial z_2}) = -\nabla_r + \frac{\mu}{m_1}\nabla_R \tag{5}$$

In order to use these in the Schroedinger equation, we need however the Laplacian operators ∇^2. We see that,

$$\nabla_1^2 = (\nabla_r + \frac{\mu}{m_2}\nabla_R)\cdot(\nabla_r + \frac{\mu}{m_2}\nabla_R) = \nabla_r^2 + (\frac{\mu}{m_2})^2\nabla_R^2 + 2\frac{\mu}{m_2}(\nabla_r\cdot\nabla_R) \tag{6}$$

$$\nabla_2^2 = (\nabla_r - \frac{\mu}{m_1}\nabla_R)\cdot(\nabla_r - \frac{\mu}{m_1}\nabla_R) = \nabla_r^2 + (\frac{\mu}{m_1})^2\nabla_R^2 - 2\frac{\mu}{m_1}(\nabla_r\cdot\nabla_R) \tag{7}$$

Recall, that the two particle time-independent Schroedinger equation reads

$$[-\frac{\hbar^2}{2}(\frac{\nabla_1^2}{m_1} + \frac{\nabla_2^2}{m_2}) + V(\vec{r_1}, \vec{r_2})]\psi(\vec{r_1}, \vec{r_2}) = E\psi(\vec{r_1}, \vec{r_2}) \tag{8}$$

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Using the derived Laplacian operators we see that,

$$\frac{\nabla_1^2}{m_1} + \frac{\nabla_2^2}{m_2} = \frac{\nabla_r^2}{\mu} + \frac{\nabla_R^2}{M} \tag{9}$$

Thus, if our potential only depends on the difference in position of the two particles, $\vec{r}$, we can write the Schroedinger equations as,

$$[-\frac{\hbar^2}{2}(\frac{\nabla_r^2}{\mu} + \frac{\nabla_R^2}{M}) + V(\vec{r})]\psi(\vec{r}, \vec{R}) = E\psi(\vec{r}, \vec{R}) \tag{10}$$

This is of course separable into the two equations,

$$-\frac{\hbar^2}{2}\frac{\nabla_R^2}{M}\psi_R = E_R\psi_R \tag{11}$$

$$[-\frac{\hbar^2}{2}\frac{\nabla_r^2}{\mu} + V(\vec{r})]\psi_r = E_r\psi_r \tag{12}$$

where $E = E_R + E_r$. We have thus reduced a two particle problem to an effective one particle problem with an overall free motion of the center of mass. In the Hydrogen atom, we have made the approximation that the center of mass motion corresponds to the proton solution, which we have chosen as static in some reference frame, and that the effective relative motion corresponds to the electron solution. This is valid, since the mass of the proton is much heavier than the mass of the electron.

2. Griffiths 6.2

Let us use the solution to the harmonic oscillator and perturb the potential by changing the spring constant $k' = (1+\epsilon)k$. Recall that the energy states are given by $E_n = \hbar\omega(n + \frac{1}{2})$, with $\omega = \sqrt{k/m}$. We can write the exact perturbed energies as,

$$E_n' = \hbar\omega(n + \frac{1}{2})\sqrt{1 + \epsilon} \tag{13}$$

Expanding in powers of ϵ, we see that,

$$E_n' = \hbar\omega(n + \frac{1}{2})[1 + \frac{\epsilon}{2} - \frac{\epsilon^2}{8} + \ldots] \tag{14}$$

Let us now approach this from perturbation theory, where it is clear that $H' = \frac{\epsilon}{2}kx^2 = \epsilon V_0(x)$. Recall, that $E_n^{(1)} = <\psi_n^{(0)}|H'|\psi_n^{(0)}>$. There are two ways to easily solve this problem. First, we see that,

$$E_n^{(1)} = \epsilon < V_0 > \tag{15}$$

For the harmonic oscillator, the virial theorem states that $< V_0 >= \frac{1}{2} < H_0 >$. Thus, it is straight forward to say,

$$E_n^{(1)} = \frac{\epsilon}{2}E_n^{(0)} \tag{16}$$

A more explicit way of solving this problem is to remember that we can write the position operator in terms of raising and lower operators, $x^2 = \frac{\hbar}{2m\omega}[a_+^2 + a_+ a_- + a_- a_+ + a_-^2]$. Then we see that

$$E_n^{(1)} = <\psi_n^{(0)}|H'|\psi_n^{(0)}> = \frac{\epsilon}{4}\hbar\omega < \psi_n^{(0)}|[2n+1]|\psi_n^{(0)}> = \frac{\epsilon}{2}E_n^{(0)} \quad (17)$$

We see that the first order perturbation in energy is the same as we would have gotten by just expanding the exact energy to first order in ϵ. Let us now calculate the first order perturbation in the wavefunction,

$$\psi_n^{(1)} = \sum_{m \neq n} \frac{<\psi_m^{(0)}|H'|\psi_n^{(0)}>}{E_n^{(0)} - E_m^{(0)}}\psi_m^{(0)} = \frac{\epsilon}{8}(\sqrt{n(n-1)}\psi_{n-2}^{(0)} - \sqrt{(n+1)(n+2)}\psi_{n+2}^{(0)})$$

(18)

The first order correction to the first two normalized states can be seen in Figure 1 and compared with their respective unperturbed states. We have used an extremely large value of $\epsilon = 0.5$ to clearly show the difference. However, such a large value would not allow us to use perturbation theory. Notice, that the wavefunctions are squeezed towards the center due to the higher potential.
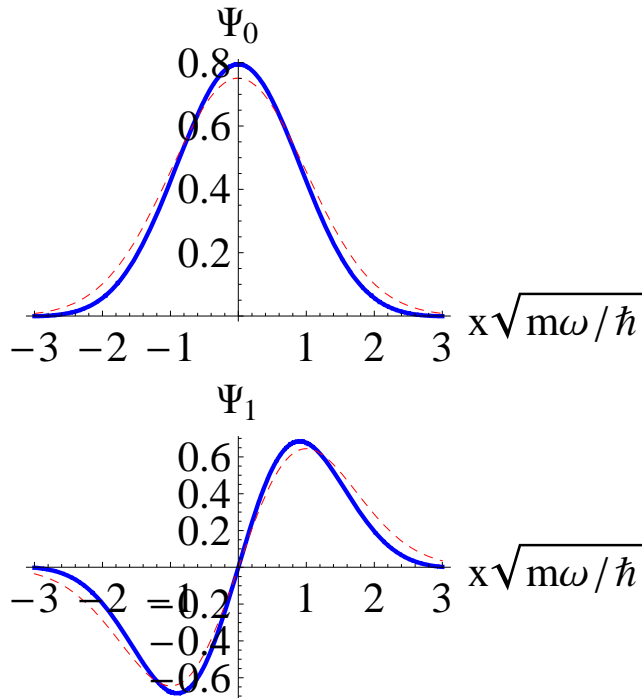

Figure 1: First order correction to the ground and first excited state of the harmonic oscillator.

3. Griffiths 6.8

Let us take an infinite cubic well, with sides of length a and perturb it with the Hamiltonian, $H' = a^3 V_0 \delta(x - a/4)\delta(y - a/2)\delta(z - 3a/4)$. Recall, that the unperturbed states are given by $\psi^{(0)}_{n_x n_y n_z} = (\frac{2}{a})^{3/2} \sin n_x \pi \frac{x}{a} \sin n_y \pi \frac{y}{a} \sin n_z \pi \frac{z}{a}$ with the energy $E^{(0)}_{n_x n_y n_z} = \frac{\pi^2 \hbar^2}{2ma^2}(n_x^2 + n_y^2 + n_z^2)$. For the ground state, which is not degenerate, we see that the perturbation in energy is,

$$E^{(1)}_{111} = <\psi^{(0)}_{111}|H'|\psi^{(0)}_{111}> = \int_{well} d^3x |\psi^{(0)}_{111}|^2 H' = 2V_0 \tag{19}$$

For the first excited states, we must use degenerate perturbation theory, and solve the eigenvalue problem $\boldsymbol{W}\phi^{(0)} = \epsilon^{(1)}\phi^{(0)}$, $W_{ij} = <\psi^{(0)}_i|H'|\psi^{(0)}_j>$. We seek to diagonalize $\boldsymbol{W}$ and obtain the "good" eigenstates, $\phi^{(0)} = \sum_D c_D \psi^{(0)}_D$, with perturbed energies, $\epsilon^{(1)}$. After some simple integrals, we find that,

$$\boldsymbol{W} = 4V_0 \begin{pmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 1 \end{pmatrix} \tag{20}$$

We thus find that the characteristic equation is

$$\epsilon^2(\epsilon - 8V_0) = 0 \tag{21}$$

Thus, the perturbed energies of the first exited states are given by $\epsilon^{(1)}_a = 0$, $\epsilon^{(1)}_b = 0$, and $\epsilon^{(1)}_c = 8V_0$. Notice, because of the location of the perturbing potential, the first excited states do not completely split. We note that the corresponding "good" eigenstates are given by $\phi^{(0)}_a = \psi^{(0)}_{121}$, $\phi^{(0)}_b = \frac{1}{\sqrt{2}}[\psi^{(0)}_{211} + \psi^{(0)}_{112}]$, and $\phi^{(0)}_c = \frac{1}{\sqrt{2}}[\psi^{(0)}_{211} - \psi^{(0)}_{112}]$.

4. Hydrogen (similar to Griffith 4.43) We are asked to construct the normalized eigenstates for Hydrogen with $n = 3$, $l = 2$, and $m = +1$. Using the Radial wavefunctions and Spherical Harmonics, we write

$$\psi_{321} = R_{32}(r)Y_2^{+1}(\theta, \phi) = -Ar^2 e^{-r/3a} \sin\theta \cos\theta e^{i\phi} \tag{22}$$

Here A is a normalization constant, which we must solve for.

$$1 = \int_{All} d^3r |\psi_{321}|^2 = |A|^2 \int_{-\infty}^{\infty} dr r^6 e^{-2r/3a} \int_0^{\pi} d\theta \sin^3\theta \cos^2\theta \int_0^{2\pi} d\phi \tag{23}$$

The integral over ϕ is trivial,

$$\int_0^{2\pi} d\phi = 2\pi \tag{24}$$

The exponential integral we find in a table,

$$\int_{-\infty}^{\infty} dr r^6 e^{-2r/3a} = 6!(\frac{3a}{2})^7 \tag{25}$$

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Finally, for θ, we use integration by parts to find,

$$\int_0^\pi d\theta \sin^3 \theta \cos^2 \theta = \frac{8}{30} \tag{26}$$

Thus, $A = (81\sqrt{\pi a^7})^{-1}$.

Using the transition rules, we see that a direct transition $\psi_{321} \to \psi_{100}$, cannot occur because the change in angular momentum can only be a maximum of one. This comes from the fact that a photon may carry spin 1 angular momentum. We can however make a two photon transition via $\psi_{321} \to \{\psi_{211}, \psi_{210}\} \to \psi_{100}$. Since the energy levels in hydrogen are described by $E_n = -13.6/n^2[eV]$, we see that the two photons will have energy, 1.9 eV (visible) and 10.2 eV (ultraviolet).