# Physics 624

## Quantum Mechanics II

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# Homework #6

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# 1 Problem #1

For a diatomic molecule where the nuclei move in a potential

$$V(r) = -2D\left(\frac{1}{\rho} - \frac{1}{2\rho^2}\right)$$

where $\rho = r/a$, $a$ is the characteristic size, this effective potential is given by

$$V_{eff}(r) = V(r) + \frac{\hbar^2}{2\mu r^2}K(K+1)$$

where $K$ is an integer. We can approximate the effective potential as a harmonic oscillator about the minimum, $r_0$, which we calculate as

$$\left.\frac{\partial V_{eff}}{\partial r}\right|_{r_0} = 0 = -2D\left(-\frac{a}{r_0^2} + \frac{a^2}{r_0^3}\right) - \frac{\hbar^2}{\mu r_0^3}K(K+1)$$
$$\Downarrow$$
$$\frac{2Da}{r_0^2} = \frac{2Da^2}{r_0^3} + \frac{\hbar^2}{\mu r_0^3}K(K+1)$$
$$\Downarrow$$
$$r_0 = a + \frac{\hbar^2}{2\mu Da}K(K+1)$$

Now we can Taylor expand the effective potential about $r_0$ to get a parabolic approximation

$$\begin{aligned}
V_{eff}(r) &= V_{eff}(r_0) + \cancelto{0}{\left.\frac{\partial V_{eff}}{\partial r}\right|_{r_0}}(r-r_0) + \frac{1}{2}\left.\frac{\partial^2 V_{eff}}{\partial r^2}\right|_{r_0}(r-r_0)^2 \\
&= V_{eff}(r_0) + \frac{1}{2}\left.\frac{\partial^2 V_{eff}}{\partial r^2}\right|_{r_0}(r-r_0)^2 \\
&\Downarrow \\
&= V_{eff}(r_0) + \frac{1}{2}\mu\omega^2(r-r_0)^2
\end{aligned}$$

Note that this approximation transformed the effective potential into a harmonic oscillator potential where

$$\begin{aligned}
\mu\omega^2 = \left.\frac{\partial^2 V_{eff}}{\partial r^2}\right|_{r_0} &= -2D\left(\frac{2a}{r_0^3} - \frac{3a^2}{r_0^4}\right) + \frac{3\hbar^2}{\mu r_0^4}K(K+1) \\
&= -4Da\left(\frac{2\mu Da}{2\mu Da^2 + \hbar^2 K(K+1)}\right)^3 + 3\frac{2\mu Da^2 + \hbar^2 K(K+1)}{\mu}\left(\frac{2\mu Da}{2\mu Da^2 + \hbar^2 K(K+1)}\right)^4 \\
&= -\frac{2}{\mu}\frac{(2\mu Da)^4}{(2\mu Da^2 + \hbar^2 K(K+1))^3} + \frac{3}{\mu}\frac{(2\mu Da)^4}{(2\mu Da^2 + \hbar^2 K(K+1))^3} \\
&\Downarrow \\
\omega &= \frac{(2\mu Da)^2}{\mu(2\mu Da^2 + \hbar^2 K(K+1))^{3/2}}
\end{aligned}$$

which gives us the energy levels

$$E = V(r_0) + \frac{\hbar^2 K(K+1)}{2I} + \frac{4\hbar\mu(Da)^2}{(2\mu Da^2 + \hbar^2 K(K+1))^{3/2}}\left(n + \frac{1}{2}\right)$$

where $I = \mu r_0^2$. Note the first two terms are constant.

## 2 Problem #2

We can use the variational method with the trial function

$$\psi = Ae^{-\beta r}$$

to find the ground state energy of the hydrogen atom with has the Hamiltonian

$$H = -\frac{\hbar^2}{2\mu}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{e^2}{r}$$

First we find $A$ by the normalization condition

$$\begin{aligned}
\int \psi^*\psi dr = 1 &= |A|^2 4\pi \int_0^\infty e^{-2\beta r} r^2 dr \\
&= |A|^2 \frac{\pi}{\beta^3} \\
&\Downarrow \\
A &= \sqrt{\frac{\beta^3}{\pi}}
\end{aligned}$$

Then using the condition of the variational method which states

$$E_0 \leq \langle\psi|H|\psi\rangle$$

so we calculate

$$\begin{aligned}
\langle\psi|H|\psi\rangle = E(\beta) &= \frac{\beta^3}{\pi}4\pi\int_0^\infty e^{-\beta r}\left(-\frac{\hbar^2}{2\mu}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{e^2}{r}\right)e^{-\beta r}r^2 dr \\
&= 4\beta^3\int_0^\infty \frac{\hbar^2}{2\mu}2\beta e^{-2\beta r}r - \frac{\hbar^2}{2\mu}\beta^2 e^{-2\beta r}r^2 - e^2 e^{-2\beta r} r dr \\
&= \frac{\hbar^2}{2\mu}\beta^2 - e^2\beta
\end{aligned}$$

Now we minimize $E(\beta)$ to find that

$$\begin{aligned}
\left.\frac{\partial E(\beta)}{\partial \beta}\right|_{\beta_0} &= 0 = \frac{\hbar^2}{\mu}\beta_0 - e^2 \\
&\Downarrow \\
\beta_0 &= \frac{e^2\mu}{\hbar^2} = \frac{1}{a}
\end{aligned}$$

where $a$ is the *Bohr Radius.* This yields the ground state energy

$$\begin{aligned}
E_0 \leq E(\beta_0) &= \frac{\hbar^2}{2\mu}\beta_0^2 - e^2\beta_0 \\
&= \frac{\hbar^2}{2\mu}\frac{e^4\mu^2}{\hbar^4} - \frac{e^4\mu}{\hbar^2} \\
&= -\frac{e^4\mu}{2\hbar^2}
\end{aligned}$$

Note that this recovers the exact result for the ground state of hydrogen. Also we see that we recover the exact ground state wave function

$$\psi(r) = \frac{1}{\sqrt{\pi a^3}}e^{-r/a}$$

# 3 Problem #3

Two particles have equal spins $s_1 = s_2 = 1$. We can find the wave function describing the states with the overall spin $S = 1$ and 2 and $S_z = +1$ and $-1$, as well as $S = 1$ and $S_z = 0$ in the $s_{1z}s_{2z}$ representation by first noting that the states with $S = 2$ and $S_z = +2$ and $-2$ in the $s_{1z}s_{2z}$ representation are

$$\Psi_{2,2} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}_1 \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}_2 \qquad \Psi_{2,-2} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}_1 \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}_2$$

Using these states we can act the ladder operators on the state where

$$\hat{L}_\pm \Psi_{S,S_z} = \sqrt{(S \mp S_z)(S \pm S_z + 1)}\Psi_{S,S_z - 1}$$

where we can take the ladder operator in $s_{1z}s_{2z}$ representation as

$$\hat{L}_\pm = \hat{L}_{1\pm} + \hat{L}_{2\pm}$$

so we can act of the state with $S = 2$ and $S_z = +2$ as

$$\hat{L}_- \Psi_{2,2} = (\hat{L}_{1-} + \hat{L}_{2-}) \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}_1 \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}_2$$

$$\Downarrow$$

$$2\Psi_{2,1} = \sqrt{2} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}_1 \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}_2 + \sqrt{2} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}_1 \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}_2$$

$$\Psi_{2,1} = \frac{1}{\sqrt{2}} \left[ \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}_1 \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}_2 + \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}_1 \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}_2 \right]$$

And by raising the $S = 2$ $S_z = -2$ state we get

$$\hat{L}_+ \Psi_{2,-2} = (\hat{L}_{1+} + \hat{L}_{2+}) \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}_1 \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}_2$$

$$\Downarrow$$

$$2\Psi_{2,-1} = \sqrt{2} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}_1 \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}_2 + \sqrt{2} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}_1 \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}_2$$

$$\Psi_{2,-1} = \frac{1}{\sqrt{2}} \left[ \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}_1 \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}_2 + \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}_1 \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}_2 \right]$$

We note that these state have parallel spins as the wave function is additive. This yields a $S = 2$ state if we make the wave function anti-parallel we can find the $S = 1$ states as

$$\Psi_{1,1} = \frac{1}{\sqrt{2}} \left[ \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}_1 \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}_2 - \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}_1 \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}_2 \right]$$

$$\Psi_{1,-1} = \frac{1}{\sqrt{2}} \left[ \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}_1 \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}_2 - \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}_1 \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}_2 \right]$$

From here we can easily find the $S = 1$ $S_z = 0$ state by using a ladder operator

$$\hat{L}_-\Psi_{1,1} = \frac{1}{\sqrt{2}}(\hat{L}_{1-} + \hat{L}_{2-})\left[\begin{pmatrix}0\\1\\0\end{pmatrix}_1\begin{pmatrix}1\\0\\0\end{pmatrix}_2 - \begin{pmatrix}1\\0\\0\end{pmatrix}_1\begin{pmatrix}0\\1\\0\end{pmatrix}_2\right]$$

$$\Downarrow$$

$$\sqrt{2}\Psi_{1,0} = \frac{1}{\sqrt{2}}\left[\sqrt{2}\begin{pmatrix}0\\0\\1\end{pmatrix}_1\begin{pmatrix}1\\0\\0\end{pmatrix}_2 - \sqrt{2}\begin{pmatrix}0\\1\\0\end{pmatrix}_1\begin{pmatrix}0\\1\\0\end{pmatrix}_2 + \sqrt{2}\begin{pmatrix}0\\1\\0\end{pmatrix}_1\begin{pmatrix}0\\1\\0\end{pmatrix}_2 - \sqrt{2}\begin{pmatrix}1\\0\\0\end{pmatrix}_1\begin{pmatrix}0\\0\\1\end{pmatrix}_2\right]$$

$$\Psi_{1,0} = \frac{1}{\sqrt{2}}\left[\begin{pmatrix}0\\0\\1\end{pmatrix}_1\begin{pmatrix}1\\0\\0\end{pmatrix}_2 - \begin{pmatrix}1\\0\\0\end{pmatrix}_1\begin{pmatrix}0\\0\\1\end{pmatrix}_2\right]$$