PHY4370 ASSIGNMENT 6

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Problem 1. Bransden and Joachain Problem 10.4

The average energy is given by

$$E = \frac{\langle \phi | H | \phi \rangle}{\langle \phi | \phi \rangle} = \langle \phi | H | \phi \rangle$$

Since ϕ is normalised. We want to compute $\int \phi^* H \phi d\mathbf{r}_1 d\mathbf{r}_2$. Since ϕ has no angular dependence we can focus on only the r part of ∇^2.

$$\begin{aligned}
\nabla_1^2 \phi &= \frac{1}{\pi}\Big(\frac{\lambda}{a_0}\Big)^3 \nabla_1^2 e^{-\frac{\lambda}{a_0}(r_1+r_2)} \\
&= \frac{1}{\pi}\Big(\frac{\lambda}{a_0}\Big)^3 \frac{1}{r_1^2}\frac{\partial}{\partial r_1}\Big(r_1^2 \frac{\partial}{\partial r_1} e^{-\frac{\lambda}{a_0}(r_1+r_2)}\Big) \\
&= \frac{1}{\pi}\Big(\frac{\lambda}{a_0}\Big)^3 \frac{1}{r_1^2}\frac{\partial}{\partial r_1}\Big(r_1^2 (\frac{-\lambda}{a_0}) e^{-\frac{\lambda}{a_0}(r_1+r_2)}\Big) \\
&= -\frac{1}{\pi}\Big(\frac{\lambda}{a_0}\Big)^4 \frac{1}{r_1^2}\frac{\partial}{\partial r_1}\Big(r_1^2 e^{-\frac{\lambda}{a_0}(r_1+r_2)}\Big) \\
&= -\frac{1}{\pi}\Big(\frac{\lambda}{a_0}\Big)^4 \frac{1}{r_1^2}\Big(2r_1 e^{-\frac{\lambda}{a_0}(r_1+r_2)} - \frac{\lambda}{a_0} r_1^2 e^{-\frac{\lambda}{a_0}(r_1+r_2)}\Big) \\
&= -\frac{1}{\pi}\Big(\frac{\lambda}{a_0}\Big)^4 \Big(2\frac{1}{r_1} e^{-\frac{\lambda}{a_0}(r_1+r_2)} - \frac{\lambda}{a_0} e^{-\frac{\lambda}{a_0}(r_1+r_2)}\Big) \\
&= -\frac{\lambda}{a_0}\Big(2\frac{1}{r_1}\frac{1}{\pi}\Big(\frac{\lambda}{a_0}\Big)^3 e^{-\frac{\lambda}{a_0}(r_1+r_2)} - \frac{\lambda}{a_0}\frac{1}{\pi}\Big(\frac{\lambda}{a_0}\Big)^3 e^{-\frac{\lambda}{a_0}(r_1+r_2)}\Big) \\
&= -\frac{\lambda}{a_0}\Big(2\frac{1}{r_1}\phi - \frac{\lambda}{a_0}\phi\Big) = -\frac{2\lambda}{a_0}\phi\frac{1}{r_1} + \frac{\lambda^2}{a_0^2}\phi
\end{aligned}$$

Similarly

$$\nabla_2^2 \phi = -\frac{2\lambda}{a_0}\phi\frac{1}{r_2} + \frac{\lambda^2}{a_0^2}\phi$$

Now

$$\begin{aligned}
H\phi &= -\frac{\hbar^2}{2m}\nabla_1^2\phi - \frac{Ze^2}{4\pi\epsilon_0 r_1}\phi - \frac{\hbar^2}{2m}\nabla_2^2\phi - \frac{Ze^2}{4\pi\epsilon_0 r_2}\phi + \frac{e^2}{4\pi\epsilon_0 r_{12}}\phi \\
&= -\frac{\hbar^2}{2m}(-\frac{2\lambda}{a_0})\phi\frac{1}{r_1} - \frac{\hbar^2}{2m}\frac{\lambda^2}{a_0^2}\phi - \frac{Ze^2}{4\pi\epsilon_0}\frac{1}{r_1}\phi - \frac{\hbar^2}{2m}(-\frac{2\lambda}{a_0})\phi\frac{1}{r_2} - \frac{\hbar^2}{2m}\frac{\lambda^2}{a_0^2}\phi - \frac{Ze^2}{4\pi\epsilon_0}\frac{1}{r_2}\phi + \frac{e^2}{4\pi\epsilon_0 r_{12}}\phi \\
&= \frac{\hbar^2\lambda}{ma_0}\frac{1}{r_1}\phi - \frac{Ze^2}{4\pi\epsilon_0}\frac{1}{r_1}\phi + \frac{\hbar^2\lambda}{ma_0}\frac{1}{r_2}\phi - \frac{Ze^2}{4\pi\epsilon_0}\frac{1}{r_2}\phi + \frac{e^2}{4\pi\epsilon_0 r_{12}}\phi - \frac{\hbar^2}{m}\frac{\lambda^2}{a_0^2}\phi \\
&= \Big(\frac{\hbar^2\lambda}{ma_0} - \frac{Ze^2}{4\pi\epsilon_0}\Big)\Big(\frac{1}{r_1}\phi + \frac{1}{r_2}\phi\Big) + \frac{e^2}{4\pi\epsilon_0 r_{12}}\phi - \frac{\hbar^2}{m}\frac{\lambda^2}{a_0^2}\phi
\end{aligned}$$

Multiplying by $\phi^* = \phi$:

$$\phi^* H \phi = \Big(\frac{\hbar^2 \lambda}{m a_0} - \frac{Z e^2}{4\pi\epsilon_0}\Big)\Big(\frac{1}{r_1}\phi^2 + \frac{1}{r_2}\phi^2\Big) + \frac{e^2}{4\pi\epsilon_0 r_{12}}\phi^2 - \frac{\hbar^2}{m}\frac{\lambda^2}{a_0^2}\phi^2$$

Integrating,

$$E = \langle\phi|H|\phi\rangle = \Big(\frac{\hbar^2 \lambda}{m a_0} - \frac{Z e^2}{4\pi\epsilon_0}\Big)\Big(\langle\phi|\frac{1}{r_1}|\phi\rangle + \langle\phi|\frac{1}{r_2}|\phi\rangle\Big) + \frac{e^2}{4\pi\epsilon_0}\langle\phi|\frac{1}{r_{12}}|\phi\rangle - \frac{\hbar^2}{m}\frac{\lambda^2}{a_0^2}\langle\phi|\phi\rangle$$

Now we evaluate each integral. $\langle\phi|\phi\rangle = 1$.

$$\begin{aligned}
\langle\phi|\frac{1}{r_1}|\phi\rangle &= \int \phi^2 \frac{1}{r_1} d\mathbf{r}_1 d\mathbf{r}_2 \\
&= \int_0^\infty \int_0^\infty \phi^2 \frac{1}{r_1} r_1^2 r_2^2 dr_1 dr_2 \int_0^\pi \sin\theta_1 d\theta_1 \int_0^\pi \sin\theta_2 d\theta_2 \int_0^{2\pi} d\phi_1 \int_0^{2\pi} d\phi_2 \\
&= \int_0^\infty r_2^2 \int_0^\infty \phi^2 r_1 dr_1 dr_2 (2)(2)(2\pi)(2\pi) \\
&= 16\pi^2 \int_0^\infty r_2^2 \int_0^\infty \phi^2 r_1 dr_1 dr_2 \\
&= 16\Big(\frac{\lambda}{a_0}\Big)^6 \int_0^\infty r_2^2 \int_0^\infty r_1 e^{-\frac{2\lambda}{a_0}(r_1+r_2)} dr_1 dr_2 \\
&= 16\Big(\frac{\lambda}{a_0}\Big)^6 \int_0^\infty r_2^2 e^{-\frac{2\lambda}{a_0}r_2} \int_0^\infty r_1 e^{-\frac{2\lambda}{a_0}r_1} dr_1 dr_2
\end{aligned}$$

To solve these integrals we can use the gamma function since $\Gamma(x) = \int_0^\infty u^{x-1}e^{-u}du$. Let $u = \frac{2\lambda}{a_0}r_1$ which implies $r_1 = \frac{a_0}{2\lambda}u$ and $dr_1 = \frac{a_0}{2\lambda}du$. Then

$$\int_0^\infty r_1 e^{-\frac{2\lambda}{a_0}r_1} dr_1 \;=\; \Big(\frac{a_0}{2\lambda}\Big)^2 \int_0^\infty u e^{-u} du = \Big(\frac{a_0}{2\lambda}\Big)^2 \Gamma(2) = \Big(\frac{a_0}{2\lambda}\Big)^2 1! = \Big(\frac{a_0}{2\lambda}\Big)^2$$

Since $\Gamma(n+1) = n!$. Similarly,

$$\int_0^\infty r_2^2 e^{-\frac{2\lambda}{a_0}r_2} dr_2 = \int_0^\infty \Big(\frac{a_0}{2\lambda}\Big)^3 u^2 e^{-u} du = \Big(\frac{a_0}{2\lambda}\Big)^3 \int_0^\infty u^2 e^{-u} du = \Big(\frac{a_0}{2\lambda}\Big)^3 \Gamma(3) = \Big(\frac{a_0}{2\lambda}\Big)^3 2! = 2\Big(\frac{a_0}{2\lambda}\Big)^3$$

Substituting this back in

$$\langle\phi|\frac{1}{r_1}|\phi\rangle = 16\Big(\frac{\lambda}{a_0}\Big)^6 2\Big(\frac{a_0}{2\lambda}\Big)^3\Big(\frac{a_0}{2\lambda}\Big)^2 = \frac{32}{8(4)}\frac{\lambda}{a_0} = \frac{\lambda}{a_0}$$

Now since $\phi(r_1, r_2) = \phi(r_2, r_1)$, the $\langle\phi|\frac{1}{r_2}|\phi\rangle$ integral goes exactly the same way and we have

$$\langle\phi|\frac{1}{r_2}|\phi\rangle = \frac{\lambda}{a_0}$$

Now we evaluate $\langle\phi|\frac{1}{r_{12}}|\phi\rangle = \int \phi^2 \frac{1}{r_{12}} d\mathbf{r}_1 d\mathbf{r}_2$ where $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$ following the way they did it in the book (p.489 eqs 10.75-10.80). The factor $\frac{1}{r_{12}}$ can be expanded as

$$\frac{1}{r_{12}} = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} \frac{4\pi}{2l+1}\frac{(r_<)^l}{(r_>)^{l+1}} Y_{lm}^*(\theta_1,\phi_1) Y_{lm}(\theta_2,\phi_2)$$

where $r_<$ is the smaller of r_1 and r_2, $r_>$ is the larger of r_1 and r_2, and $Y_{lm}(\theta,\phi)$ is the spherical harmonic function. Substitute this expansion and we get

$$
\begin{aligned}
\langle\phi|\frac{1}{r_{12}}|\phi\rangle &= \sum_{l=0}^{\infty}\sum_{m=-l}^{l}\frac{4\pi}{2l+1}\int \phi^2\frac{(r_<)^l}{(r_>)^{l+1}}Y_{lm}^*(\theta_1,\phi_1)Y_{lm}(\theta_2,\phi_2)d\mathbf{r}_1 d\mathbf{r}_2 \\
&= \sum_{l=0}^{\infty}\sum_{m=-l}^{l}\frac{4\pi}{2l+1}\int_0^\infty r_1^2\int_0^\infty r_2^2\phi^2\frac{(r_<)^l}{(r_>)^{l+1}}dr_2dr_1\int Y_{lm}^*(\theta_1,\phi_1)d\Omega_1\int Y_{lm}(\theta_2,\phi_2)d\Omega_2 \\
&= \sum_{l=0}^{\infty}\sum_{m=-l}^{l}\frac{4\pi}{2l+1}\frac{4\pi}{4\pi}\int_0^\infty r_1^2\int_0^\infty r_2^2\phi^2\frac{(r_<)^l}{(r_>)^{l+1}}dr_2dr_1\int Y_{lm}^*(\theta_1,\phi_1)d\Omega_1\int Y_{lm}(\theta_2,\phi_2)d\Omega_2
\end{aligned}
$$

Note that $Y_{00}(\theta,\phi)=\frac{1}{\sqrt{4\pi}}$. So

$$
\langle\phi|\frac{1}{r_{12}}|\phi\rangle = \sum_{l=0}^{\infty}\sum_{m=-l}^{l}\frac{16\pi^2}{2l+1}\int_0^\infty r_1^2\int_0^\infty r_2^2\phi^2\frac{(r_<)^l}{(r_>)^{l+1}}dr_2dr_1\int Y_{lm}^*(\theta_1,\phi_1)Y_{00}d\Omega_1\int Y_{00}Y_{lm}(\theta_2,\phi_2)d\Omega_2
$$

Since the spherical harmonic functions are orthogonal we have

$$
\langle\phi|\frac{1}{r_{12}}|\phi\rangle = \sum_{l=0}^{\infty}\sum_{m=-l}^{l}\frac{16\pi^2}{2l+1}\int_0^\infty r_1^2\int_0^\infty r_2^2\phi^2\frac{(r_<)^l}{(r_>)^{l+1}}dr_2dr_1\delta_{0l}\delta_{0m}
$$

Which means that $l=m=0$. So

$$
\begin{aligned}
\langle\phi|\frac{1}{r_{12}}|\phi\rangle &= 16\pi^2\int_0^\infty r_1^2\int_0^\infty r_2^2\phi^2\frac{1}{r_>}dr_2dr_1 \\
&= 16\Big(\frac{\lambda}{a_0}\Big)^6\int_0^\infty r_1^2\int_0^\infty r_2^2 e^{-\frac{2\lambda}{a_0}(r_1+r_2)}\frac{1}{r_>}dr_2dr_1 \\
&= 16\Big(\frac{\lambda}{a_0}\Big)^6\int_0^\infty r_1^2 e^{-\frac{2\lambda}{a_0}r_1}\int_0^\infty r_2^2 e^{-\frac{2\lambda}{a_0}r_2}\frac{1}{r_>}dr_2dr_1
\end{aligned}
$$

Now we evaluate $\int_0^\infty r_2^2 e^{-\frac{2\lambda}{a_0}r_2}\frac{1}{r_>}dr_2$.

$$
\begin{aligned}
\int_0^\infty r_2^2 e^{-\frac{2\lambda}{a_0}r_2}\frac{1}{r_>}dr_2 &= \int_0^{r_1}\frac{1}{r_1}r_2^2 e^{-\frac{2\lambda}{a_0}r_2}dr_2+\int_{r_1}^\infty\frac{1}{r_2}r_2^2 e^{-\frac{2\lambda}{a_0}r_2}dr_2 \\
&= \frac{1}{r_1}\int_0^{r_1}r_2^2 e^{-\frac{2\lambda}{a_0}r_2}dr_2+\int_{r_1}^\infty r_2 e^{-\frac{2\lambda}{a_0}r_2}dr_2
\end{aligned}
$$

These can be solved by integrating by parts. For $\int_{r_1}^\infty r_2 e^{-\frac{2\lambda}{a_0}r_2}dr_2$ use $u=r_2$ and $dv=e^{-\frac{2\lambda}{a_0}r_2}dr_2$.

$$
\begin{aligned}
\int_{r_1}^\infty r_2 e^{-\frac{2\lambda}{a_0}r_2}dr_2 &= -\frac{a_0}{2\lambda}r_2 e^{-\frac{2\lambda}{a_0}r_2}+\frac{a_0}{2\lambda}\int_{r_1}^\infty e^{-\frac{2\lambda}{a_0}r_2}dr_2 \\
&= -\frac{a_0}{2\lambda}r_2 e^{-\frac{2\lambda}{a_0}r_2}-\Big(\frac{a_0}{2\lambda}\Big)^2 e^{-\frac{2\lambda}{a_0}r_2}\Big|_{r_1}^\infty \\
&= \frac{a_0}{2\lambda}r_1 e^{-\frac{2\lambda}{a_0}r_1}+\Big(\frac{a_0}{2\lambda}\Big)^2 e^{-\frac{2\lambda}{a_0}r_1} \qquad \text{since } \lim_{x\to\infty}xe^{-x}=0
\end{aligned}
$$

For $\int_0^{r_1} r_2^2 e^{-\frac{2\lambda}{a_0}r_2} dr_2$ use $u = r_2^2$ and $dv = e^{-\frac{2\lambda}{a_0}r_2} dr_2$.

$$\begin{aligned}
\int_0^{r_1} r_2^2 e^{-\frac{2\lambda}{a_0}r_2} dr_2 &= -\Big(\frac{a_0}{2\lambda}\Big) r_2^2 e^{-\frac{2\lambda}{a_0}r_2} + \frac{a_0}{\lambda}\int_0^{r_1} r_2 e^{-\frac{2\lambda}{a_0}r_2} dr_2 \\
&= -\Big(\frac{a_0}{2\lambda}\Big) r_2^2 e^{-\frac{2\lambda}{a_0}r_2} + \frac{a_0}{\lambda}\Big[-\frac{a_0}{2\lambda} r_2 e^{-\frac{2\lambda}{a_0}r_2} - \Big(\frac{a_0}{2\lambda}\Big)^2 e^{-\frac{2\lambda}{a_0}r_2}\Big]\Big|_0^{r_1} \\
&= -\Big(\frac{a_0}{2\lambda}\Big) r_2^2 e^{-\frac{2\lambda}{a_0}r_2} - \frac{1}{2}\Big(\frac{a_0}{\lambda}\Big)^2 r_2 e^{-\frac{2\lambda}{a_0}r_2} - \frac{1}{4}\Big(\frac{a_0}{\lambda}\Big)^3 e^{-\frac{2\lambda}{a_0}r_2}\Big|_0^{r_1} \\
&= -\Big(\frac{a_0}{2\lambda}\Big) r_1^2 e^{-\frac{2\lambda}{a_0}r_1} - \frac{1}{2}\Big(\frac{a_0}{\lambda}\Big)^2 r_1 e^{-\frac{2\lambda}{a_0}r_1} - \frac{1}{4}\Big(\frac{a_0}{\lambda}\Big)^3 e^{-\frac{2\lambda}{a_0}r_1} + \frac{1}{4}\Big(\frac{a_0}{\lambda}\Big)^3 \\
\frac{1}{r_1}\int_0^{r_1} r_2^2 e^{-\frac{2\lambda}{a_0}r_2} dr_2 &= -\Big(\frac{a_0}{2\lambda}\Big) r_1 e^{-\frac{2\lambda}{a_0}r_1} - \frac{1}{2}\Big(\frac{a_0}{\lambda}\Big)^2 e^{-\frac{2\lambda}{a_0}r_1} - \frac{1}{4}\Big(\frac{a_0}{\lambda}\Big)^3 \frac{1}{r_1} e^{-\frac{2\lambda}{a_0}r_1} + \frac{1}{4}\frac{1}{r_1}\Big(\frac{a_0}{\lambda}\Big)^3
\end{aligned}$$

Putting it together

$$\begin{aligned}
\int_0^{\infty} r_2^2 e^{-\frac{2\lambda}{a_0}r_2} \frac{1}{r_>} dr_2 &= -\Big(\frac{a_0}{2\lambda}\Big) r_1 e^{-\frac{2\lambda}{a_0}r_1} - \frac{1}{2}\Big(\frac{a_0}{\lambda}\Big)^2 e^{-\frac{2\lambda}{a_0}r_1} - \frac{1}{4}\Big(\frac{a_0}{\lambda}\Big)^3 \frac{1}{r_1} e^{-\frac{2\lambda}{a_0}r_1} + \frac{1}{4}\frac{1}{r_1}\Big(\frac{a_0}{\lambda}\Big)^3 + \frac{a_0}{2\lambda} r_1 e^{-\frac{2\lambda}{a_0}r_1} \\
&\quad + \Big(\frac{a_0}{2\lambda}\Big)^2 e^{-\frac{2\lambda}{a_0}r_1} \\
&= -\frac{1}{2}\Big(\frac{a_0}{\lambda}\Big)^2 e^{-\frac{2\lambda}{a_0}r_1} - \frac{1}{4}\Big(\frac{a_0}{\lambda}\Big)^3 \frac{1}{r_1} e^{-\frac{2\lambda}{a_0}r_1} + \frac{1}{4}\frac{1}{r_1}\Big(\frac{a_0}{\lambda}\Big)^3 + \Big(\frac{a_0}{2\lambda}\Big)^2 e^{-\frac{2\lambda}{a_0}r_1} \\
&= -\Big(\frac{a_0}{2\lambda}\Big)^2 e^{-\frac{2\lambda}{a_0}r_1} - \frac{1}{4}\Big(\frac{a_0}{\lambda}\Big)^3 \frac{1}{r_1} e^{-\frac{2\lambda}{a_0}r_1} + \frac{1}{4}\frac{1}{r_1}\Big(\frac{a_0}{\lambda}\Big)^3
\end{aligned}$$

Continuing on

$$\begin{aligned}
\langle\phi|\frac{1}{r_{12}}|\phi\rangle &= 16\Big(\frac{\lambda}{a_0}\Big)^6 \int_0^{\infty} r_1^2 e^{-\frac{2\lambda}{a_0}r_1} \int_0^{\infty} r_2^2 e^{-\frac{2\lambda}{a_0}r_2} \frac{1}{r_>} dr_2 dr_1 \\
&= 16\Big(\frac{\lambda}{a_0}\Big)^6 \int_0^{\infty} r_1^2 e^{-\frac{2\lambda}{a_0}r_1} \Big(-\Big(\frac{a_0}{2\lambda}\Big)^2 e^{-\frac{2\lambda}{a_0}r_1} - \frac{1}{4}\Big(\frac{a_0}{\lambda}\Big)^3 \frac{1}{r_1} e^{-\frac{2\lambda}{a_0}r_1} + \frac{1}{4}\frac{1}{r_1}\Big(\frac{a_0}{\lambda}\Big)^3\Big) dr_1 \\
&= 16\Big(\frac{\lambda}{a_0}\Big)^6 \Big[-\Big(\frac{a_0}{2\lambda}\Big)^2 \int_0^{\infty} r_1^2 e^{-\frac{4\lambda}{a_0}r_1} dr_1 - \frac{1}{4}\Big(\frac{a_0}{\lambda}\Big)^3 \int_0^{\infty} r_1 e^{-\frac{4\lambda}{a_0}r_1} dr_1 + \frac{1}{4}\Big(\frac{a_0}{\lambda}\Big)^3 \int_0^{\infty} r_1 e^{-\frac{2\lambda}{a_0}r_1} dr_1 \Big]
\end{aligned}$$

For each integral subsitute u for the positive part of the exponent and then use the Gamma function.

$$\begin{aligned}
\langle\phi|\frac{1}{r_{12}}|\phi\rangle &= 16\Big(\frac{\lambda}{a_0}\Big)^6 \Big[-\Big(\frac{a_0}{2\lambda}\Big)^2 \Big(\frac{a_0}{4\lambda}\Big)^3 \int_0^{\infty} u^2 e^{-u} du - \frac{1}{4}\Big(\frac{a_0}{\lambda}\Big)^3 \Big(\frac{a_0}{4\lambda}\Big)^2 \int_0^{\infty} u e^{-u} du + \frac{1}{4}\Big(\frac{a_0}{\lambda}\Big)^3 \Big(\frac{a_0}{2\lambda}\Big)^2 \int_0^{\infty} u e^{-u} du \Big] \\
&= 16\Big(\frac{\lambda}{a_0}\Big)^6 \Big[-\Big(\frac{a_0}{2\lambda}\Big)^2 \Big(\frac{a_0}{4\lambda}\Big)^3 \Gamma(3) - \frac{1}{4}\Big(\frac{a_0}{\lambda}\Big)^3 \Big(\frac{a_0}{4\lambda}\Big)^2 \Gamma(2) + \frac{1}{4}\Big(\frac{a_0}{\lambda}\Big)^3 \Big(\frac{a_0}{2\lambda}\Big)^2 \Gamma(2) \Big] \\
&= 16\Big(\frac{\lambda}{a_0}\Big)^6 \Big[-2\Big(\frac{a_0}{2\lambda}\Big)^2 \Big(\frac{a_0}{4\lambda}\Big)^3 - \frac{1}{4}\Big(\frac{a_0}{\lambda}\Big)^3 \Big(\frac{a_0}{4\lambda}\Big)^2 + \frac{1}{4}\Big(\frac{a_0}{\lambda}\Big)^3 \Big(\frac{a_0}{2\lambda}\Big)^2 \Big] \\
&= 16\Big[-2\Big(\frac{\lambda}{a_0}\Big)^6 \Big(\frac{a_0}{2\lambda}\Big)^2 \Big(\frac{a_0}{4\lambda}\Big)^3 - \frac{1}{4}\Big(\frac{\lambda}{a_0}\Big)^6 \Big(\frac{a_0}{\lambda}\Big)^3 \Big(\frac{a_0}{4\lambda}\Big)^2 + \frac{1}{4}\Big(\frac{\lambda}{a_0}\Big)^6 \Big(\frac{a_0}{\lambda}\Big)^3 \Big(\frac{a_0}{2\lambda}\Big)^2 \Big] \\
&= 16\Big[-\frac{2}{4(4^3)}\frac{\lambda}{a_0} - \frac{1}{4(16)}\frac{\lambda}{a_0} + \frac{1}{4(4)}\frac{\lambda}{a_0} \Big] \\
&= -\frac{2}{16}\frac{\lambda}{a_0} - \frac{1}{4}\frac{\lambda}{a_0} + \frac{\lambda}{a_0} = (1 - \frac{1}{8} - \frac{1}{4})\frac{\lambda}{a_0} = \frac{5}{8}\frac{\lambda}{a_0}
\end{aligned}$$

We've evaluated all the integrals we wanted. Now

$$
\begin{aligned}
E &= \Big(\frac{\hbar^2\lambda}{ma_0} - \frac{Ze^2}{4\pi\epsilon_0}\Big)\Big(\langle\phi|\frac{1}{r_1}|\phi\rangle + \langle\phi|\frac{1}{r_2}|\phi\rangle\Big) + \frac{e^2}{4\pi\epsilon_0}\langle\phi|\frac{1}{r_{12}}|\phi\rangle - \frac{\hbar^2}{m}\frac{\lambda^2}{a_0^2}\langle\phi|\phi\rangle \\
&= \Big(\frac{\hbar^2\lambda}{ma_0} - \frac{Ze^2}{4\pi\epsilon_0}\Big)\Big(\frac{2\lambda}{a_0}\Big) + \frac{e^2}{4\pi\epsilon_0}\frac{5}{8}\frac{\lambda}{a_0} - \frac{\hbar^2}{m}\frac{\lambda^2}{a_0^2} \\
&= \frac{\lambda}{a_0}\Big(\frac{2\hbar^2\lambda}{ma_0} - 2Z\frac{e^2}{4\pi\epsilon_0} + \frac{5}{8}\frac{e^2}{4\pi\epsilon_0} - \frac{\hbar^2\lambda}{ma_0}\Big) \\
&= \frac{\lambda}{a_0}\Big(\frac{\hbar^2\lambda}{ma_0} - 2Z\frac{e^2}{4\pi\epsilon_0} + \frac{5}{8}\frac{e^2}{4\pi\epsilon_0}\Big) \\
&= \frac{\lambda}{a_0}\Big(\lambda\frac{e^2}{4\pi\epsilon_0} - 2Z\frac{e^2}{4\pi\epsilon_0} + \frac{5}{8}\frac{e^2}{4\pi\epsilon_0}\Big) \qquad \text{using } a_0 = \frac{4\pi\epsilon_0\hbar^2}{me^2} \\
&= \frac{e^2}{4\pi\epsilon_0(a_0)}\Big(\lambda^2 - 2Z\lambda + \frac{5}{8}\lambda\Big)
\end{aligned}
$$

as wanted.

Now we want to find λ such that E is minimized. This is given by

$$
\begin{aligned}
0 &= \frac{dE}{d\lambda} = \frac{e^2}{4\pi\epsilon_0(a_0)}\Big(2\lambda - 2Z + \frac{5}{8}\Big) \\
0 &= 2\lambda - 2Z + \frac{5}{8} \\
\lambda &= Z + \frac{5}{16}
\end{aligned}
$$

QED

Problem 2. Energy Levels of a multi-particle system.

(a) Consider a system of three independent electrons whose Hamiltonian can be written $H = h_0(1) + h_0(2) + h_0(3)$. Find the energy levels of H and their degrees of degeneracy.

I assume the electrons are distinguishable, and I find the degrees of degeneracy in orbital space.

The wavefunction for the system is the product of the individual wavefunctions of each particle (since the particles are distinguishable) and the energy levels of H are the sums of the individual energies of the particles. There are three non-degenerate eigenstates a, b, and c, each electron can be in, and the energies of the three states are 0, $\hbar\omega_0$, and $2\hbar\omega_0$, respectively. Since the electrons are independent they can occupy the same state without violating the Pauli Exclusion principle. Moreover we can distinguish which particle is in which state. So there are $3^3 = 27$ possible states.

Energy Level of H	Possible State ($e_1e_2e_3$)	Degeneracy in Orbital Space
$6\hbar\omega_0$	(ccc)	1
$5\hbar\omega_0$	$(bcc), (cbc), (ccb)$	3
$4\hbar\omega_0$	$(acc), (bbc), (bcb), (cbb), (cac), (cca)$	6
$3\hbar\omega_0$	$(abc), (acb), (bac), (bbb), (bca), (cab), (cba)$	7
$2\hbar\omega_0$	$(aac), (abb), (aca), (bab), (bba), (caa)$	6
$1\hbar\omega_0$	$(aab), (aba), (baa)$	3
$0\hbar\omega_0$	(aaa)	1

Table 1. Independent Electrons

(b) Same question for a system of three identical bosons of spin 0.

Here the bosons are indistinguishable. Their wavefunction is the totally symmetric wavefunction. Because they are bosons they can share the same state (there is no exclusion principle). We cannot distinguish which particle is in which state, so for example the system states bcc, cbc, ccb are indistinguishable and count as 1 state. In this case I'll write $1b2c$ to mean 1 particle is in the b state while the other two are in the c state.

Energy Level of H	Possible State $(e_1e_2e_3)$	Degeneracy in Orbital Space
$6\hbar\omega_0$	$3c$	1
$5\hbar\omega_0$	$1b2c$	1
$4\hbar\omega_0$	$1a2c$, $1c2b$	2
$3\hbar\omega_0$	$1a1b1c$, $3b$	2
$2\hbar\omega_0$	$2a1c$, $1a2b$	2
$1\hbar\omega_0$	$2a1b$	1
$0\hbar\omega_0$	$3a$	1

TABLE 2. Identical Bosons

Problem 3. Two-Electron System

(a) Construct a properly normalized two-electron wave function. Both electrons share the same spin state.

Since electrons are fermions the system is described by a totally antisymmetric wavefunction. The problem is 1dimensional so the two electrons are described by a position x_1 and x_2 respectively.

$$\psi(x_1, x_2) = \frac{1}{\sqrt{2}}[u_\alpha(x_1)u_\beta(x_2) - u_\alpha(x_2)u_\beta(x_1)]$$

Where u_α and u_β are the individual wavefunctions, given by

$$\begin{aligned} u_\alpha(x_1) &= \sqrt{\frac{\mu}{\pi}}e^{-\frac{\mu}{2}(x_1-a)^2} \\ u_\beta(x_2) &= \sqrt{\frac{\mu}{\pi}}e^{-\frac{\mu}{2}(x_2+a)^2} \end{aligned}$$

where a is a constant. So

$$\psi(x_1, x_2) = A\frac{1}{\sqrt{2}}\frac{\mu}{\pi}\left(e^{-\frac{\mu}{2}(x_1-a)^2}e^{-\frac{\mu}{2}(x_2+a)^2} - e^{-\frac{\mu}{2}(x_2-a)^2}e^{-\frac{\mu}{2}(x_1+a)^2}\right)$$

and A is a normalization constant.

To normalize it,

$$\begin{aligned} |\psi|^2 &= A^2\frac{\mu^2}{2\pi^2}\left(e^{-\frac{\mu}{2}(x_1-a)^2}e^{-\frac{\mu}{2}(x_2+a)^2} - e^{-\frac{\mu}{2}(x_2-a)^2}e^{-\frac{\mu}{2}(x_1+a)^2}\right)^2 \\ &= A^2\frac{\mu^2}{2\pi^2}\left(e^{-\mu(x_1-a)^2}e^{-\mu(x_2+a)^2} + e^{-\mu(x_2-a)^2}e^{-\mu(x_1+a)^2} - e^{-\frac{\mu}{2}(x_1-a)^2}e^{-\frac{\mu}{2}(x_2+a)^2}e^{-\frac{\mu}{2}(x_2-a)^2}e^{-\frac{\mu}{2}(x_1+a)^2}\right) \end{aligned}$$

Now

$$\begin{aligned} 1 &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}|\psi^2|dx_1dx_2 \\ &= A^2\frac{\mu^2}{2\pi^2}\left[\int_{-\infty}^{\infty}e^{-\mu(x_1-a)^2}dx_1\int_{-\infty}^{\infty}e^{-\mu(x_2+a)^2}dx_2 + \int_{-\infty}^{\infty}e^{-\mu(x_2-a)^2}dx_1\int_{-\infty}^{\infty}e^{-\mu(x_1+a)^2}dx_2\right. \\ &\quad \left. - \int_{-\infty}^{\infty}e^{-\frac{\mu}{2}(x_1-a)^2}e^{-\frac{\mu}{2}(x_1+a)^2}dx_1\int_{-\infty}^{\infty}e^{-\frac{\mu}{2}(x_2+a)^2}e^{-\frac{\mu}{2}(x_2-a)^2}dx_2\right] \\ &= A^2\frac{\mu^2}{2\pi^2}\left[\frac{\pi}{\mu} + \frac{\pi}{\mu} - \int_{-\infty}^{\infty}e^{-\frac{\mu}{2}(x_1-a)^2}e^{-\frac{\mu}{2}(x_1+a)^2}dx_1\int_{-\infty}^{\infty}e^{-\frac{\mu}{2}(x_2+a)^2}e^{-\frac{\mu}{2}(x_2-a)^2}dx_2\right] \end{aligned}$$

The exponents in the last two integrals work out to a gaussian:

$$-\frac{\mu}{2}\Big((x_1-a)^2+(x_1+a)^2\Big) = -\frac{\mu}{2}(x_1^2-2ax_1+a^2+x_1^2+2ax_1+a^2) = -\mu(x_1^2+a^2)$$

So

$$\begin{aligned}
\int_{-\infty}^{\infty} e^{-\frac{\mu}{2}(x_1-a)^2}e^{-\frac{\mu}{2}(x_1+a)^2}dx_1 &= \int_{-\infty}^{\infty} e^{-\mu(x_1^2+a^2)}dx_1 \\
&= e^{-\mu a^2}\int_{-\infty}^{\infty} e^{-\mu x_1^2}dx_1 \\
&= e^{-\mu a^2}\sqrt{\frac{\pi}{\mu}} \\
&= \int_{-\infty}^{\infty} e^{-\frac{\mu}{2}(x_2+a)^2}e^{-\frac{\mu}{2}(x_2-a)^2}dx_2
\end{aligned}$$

So

$$\begin{aligned}
1 &= A^2\frac{\mu^2}{2\pi^2}\Big(2\frac{\pi}{\mu}-e^{-2\mu a^2}\frac{\pi}{\mu}\Big) \\
1 &= A^2\frac{1}{2}\frac{\mu}{\pi}(2-e^{-2\mu a^2}) \\
A^2 &= \frac{2\pi}{\mu}\frac{1}{2-e^{-2\mu a^2}} \\
A &= \sqrt{\frac{2\pi}{\mu(2-e^{-2\mu a^2})}}
\end{aligned}$$

So the wavefunction is

$$\psi(x_1,x_2) = \sqrt{\frac{\mu}{\pi(2-e^{-2\mu a^2})}}\Big(e^{-\frac{\mu}{2}(x_1-a)^2}e^{-\frac{\mu}{2}(x_2+a)^2} - e^{-\frac{\mu}{2}(x_2-a)^2}e^{-\frac{\mu}{2}(x_1+a)^2}\Big)$$

(b) Calculate the probability that the separation between the two electrons is in the range $(x,\, x+dx)$.

The center of mass variable is $X=(x_1+x_2)/2$ and the separation is $x=x_1-x_2$. This means that

$$\begin{aligned}
x_1 &= \frac{x}{2}+X \\
x_2 &= -\frac{x}{2}+X
\end{aligned}$$

Substitute these values into $\psi(x_1,x_2)$ to get $\psi(x,X)$:

$$\begin{aligned}
\psi(x_1,x_2) &= \sqrt{\frac{\mu}{\pi(2-e^{-2\mu a^2})}}\Big(e^{-\frac{\mu}{2}(\frac{x}{2}+X-a)^2}e^{-\frac{\mu}{2}(X-\frac{x}{2}+a)^2} - e^{-\frac{\mu}{2}(X-\frac{x}{2}-a)^2}e^{-\frac{\mu}{2}(\frac{x}{2}+X+a)^2}\Big) \\
&= \psi(x,X)
\end{aligned}$$

The probability is given by $|\psi(x,X)|^2dx$.

$$\begin{aligned}
|\psi(x,X)|^2dx &= \frac{\mu}{\pi(2-e^{-2\mu a^2})}\Big(e^{-\frac{\mu}{2}(\frac{x}{2}+X-a)^2}e^{-\frac{\mu}{2}(X-\frac{x}{2}+a)^2} - e^{-\frac{\mu}{2}(X-\frac{x}{2}-a)^2}e^{-\frac{\mu}{2}(\frac{x}{2}+X+a)^2}\Big)^2dx \\
&= \frac{\mu}{\pi(2-e^{-2\mu a^2})}\Big(e^{-\mu(\frac{x}{2}+X-a)^2}e^{-\mu(X-\frac{x}{2}+a)^2} + e^{-\mu(X-\frac{x}{2}-a)^2}e^{-\mu(\frac{x}{2}+X+a)^2} \\
&\quad -e^{-\frac{\mu}{2}(\frac{x}{2}+X-a)^2}e^{-\frac{\mu}{2}(X-\frac{x}{2}+a)^2}e^{-\frac{\mu}{2}(X-\frac{x}{2}-a)^2}e^{-\frac{\mu}{2}(\frac{x}{2}+X+a)^2}\Big)dx
\end{aligned}$$