

Ψ_1

$$\rightarrow \overset{i}{\circ}, \quad \Psi_1^* \rightarrow \overset{j}{\circ}$$

 Ψ_2

$$\rightarrow \overset{i}{\circ}, \quad \Psi_2^* \rightarrow \overset{j}{\circ}$$

$$\times \begin{cases} b_i = c_1 \\ b_j = c_2 \end{cases}$$

$$a_i = b_1$$

$$a_j = b_2$$

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$$\Psi = \Psi_1 + \Psi_2$$

$$\Psi_1 = \sum_i c_i e^{-q_i(\bar{r}_1^2 + \bar{r}_2^2)}, \quad \Psi_2 = \sum_j d_j (\bar{r}_1^2 + \bar{r}_2^2) e^{-b_j(\bar{r}_1^2 + \bar{r}_2^2)}$$

$$\text{Norm} \quad \int \psi^* \psi d^3 \bar{r}_1 = \int (\Psi_1^2 + \Psi_2^2 + \Psi_1^* \Psi_2 + \Psi_2^* \Psi_1) d^3 \bar{r}_1$$

$$\Psi_1^2 = \int d^3 \bar{r}_1 e^{-2(a_i + a_j) \bar{r}_1^2}$$

$$= \left[\frac{\pi}{2(a_i + a_j)} \right]^{3/2} (d + b_i)^{1/2} (d + b_j)^{1/2}$$

$$\Psi_2^2 = \int d^3 \bar{r}_1 2 \bar{r}_1^2 e^{-2(b_i + b_j) \bar{r}_1^2}$$

$$= 4 \int d^3 \bar{r}_1 \left(\bar{r}_{1x}^2 + \bar{r}_{1y}^2 + \bar{r}_{1z}^2 \right)^2 e^{-2(b_i + b_j) \bar{r}_{1x}^2}$$

$$= 4 \int d^3 \bar{r}_1 \left(\bar{r}_{1x}^4 + \bar{r}_{1y}^4 + \bar{r}_{1z}^4 + 2 \bar{r}_{1x}^2 \bar{r}_{1y}^2 + 2 \bar{r}_{1y}^2 \bar{r}_{1z}^2 + 2 \bar{r}_{1x}^2 \bar{r}_{1z}^2 \right) e^{-2(b_i + b_j) \bar{r}_{1x}^2}$$

$$e^{-2(b_i + b_j) \bar{r}_{1x}^2} e^{-2(b_i + b_j) \bar{r}_{1y}^2} e^{-2(b_i + b_j) \bar{r}_{1z}^2}$$

$$= 4 \int d^3 \bar{r}_1 \left[\sqrt{\frac{\pi}{2(b_i + b_j)}} \left[\frac{3!}{4(b_i + b_j)} \right]^2 + \frac{2(\bar{r}_{1y}^2 + \bar{r}_{1z}^2)}{4(b_i + b_j)} \sqrt{\frac{\pi}{2(b_i + b_j)}} \right. \\ \left. + (\bar{r}_{1y}^4 + \bar{r}_{1z}^4 + 2 \bar{r}_{1y}^2 \bar{r}_{1z}^2) \sqrt{\frac{\pi}{2(b_i + b_j)}} \right]$$

①

$$= 4 \sqrt{\frac{\pi}{2(b_i+b_j)}} \left(\left[\frac{6}{16(b_i+b_j)^2} + \frac{(\bar{\tau}_{1y}^2 + \bar{\tau}_{1z}^2)}{2(b_i+b_j)} \right. \right.$$

$$\left. \left. + \bar{\tau}_{1y}^4 + \bar{\tau}_{1z}^4 + 2\bar{\tau}_{1y}^2 \bar{\tau}_{1z}^2 \right] d^3 \bar{\tau}_1 e^{-2(b_i+b_j)\bar{\tau}_{1y}^2} e^{-2(b_i+b_j)\bar{\tau}_{1z}^2} \right)$$

$$= 4 \sqrt{\frac{\pi}{2(b_i+b_j)}} \left(\left[\frac{3}{8(b_i+b_j)^2} + \frac{\bar{\tau}_{1z}^2}{2(b_i+b_j)} \right. \right.$$

$$\left. \left. + \bar{\tau}_{1y}^4 + \bar{\tau}_{1y}^2 \left(\frac{1}{2(b_i+b_j)} + 2\bar{\tau}_{1z}^2 \right) \right] e^{-2(b_i+b_j)\bar{\tau}_{1y}^2} e^{-2(b_i+b_j)\bar{\tau}_{1z}^2} \right)$$

$$= 4 \left(\frac{\pi}{2(b_i+b_j)} \right) \left[\frac{3}{8(b_i+b_j)^2} + \frac{\bar{\tau}_{1z}^2}{2(b_i+b_j)} + \bar{\tau}_{1z}^4 \right.$$

$$\left. + \frac{3}{8(b_i+b_j)^2} + \frac{1}{8(b_i+b_j)^2} + \frac{2\bar{\tau}_{1z}^2}{2(b_i+b_j)} \right] e^{-2(b_i+b_j)\bar{\tau}_{1z}^2}$$

$$= 4 \left(\frac{\pi}{2(b_i+b_j)} \right) \left[\frac{7}{8(b_i+b_j)^2} + \bar{\tau}_{1z}^4 + \frac{\bar{\tau}_{1z}^2}{(b_i+b_j)} \right] e^{-2(b_i+b_j)\bar{\tau}_{1z}^2}$$

$$= 4 \left(\frac{\pi}{2(b_i+b_j)} \right)^{3/2} \left[\frac{7}{8(b_i+b_j)^2} + \frac{1}{8(b_i+b_j)^2} + \frac{3}{8(b_i+b_j)^2} \right]$$

$$= \frac{3\sqrt{4}}{2} \left(\frac{\pi}{2(b_i+b_j)} \right)^{3/2} \frac{1}{(b_i+b_j)^2} = \frac{6}{2\sqrt{2}} \left(\frac{\pi}{b_i+b_j} \right)^{3/2} \frac{1}{(b_i+b_j)^2}$$

$$= \frac{3}{\sqrt{2}} \left(\frac{\pi^{3/2}}{(b_i+b_j)^{7/2}} \right)$$

$$\textcircled{2} \quad \frac{\frac{10}{84} + \frac{1}{4}}{\frac{6}{4\sqrt{2}}}$$

$$\begin{aligned}
\int \psi_1^* \psi_2 d^3 \bar{r}_1 &= \int (\bar{r}_1^2 + \bar{r}_2^2) e^{-(a_i + b_i)(\bar{r}_1 + \bar{r}_2)} d^3 \bar{r}_1 \\
&= 2 \int \bar{r}_1^2 e^{-2(a_i + b_i)\bar{r}_1} d\bar{r}_{1x} d\bar{r}_{1y} d\bar{r}_{1z} \\
&= 2 \int (\bar{r}_{1x}^2 + \bar{r}_{1y}^2 + \bar{r}_{1z}^2) e^{-2(a_i + b_i)\bar{r}_{1x}} e^{-2(a_i + b_i)\bar{r}_{1z}} d^3 \bar{r}_1 \\
&= 2 \left[\sqrt{\frac{\pi}{2(a_i + 2b_i)}} \frac{1}{4(a_i + b_i)} + (\bar{r}_{1y}^2 + \bar{r}_{1z}^2) \sqrt{\frac{\pi}{2(a_i + 2b_i)}} \right] e^{-2(a_i + b_i)\bar{r}_{1y}} e^{-2(a_i + b_i)\bar{r}_{1z}} \\
&= 2 \sqrt{\frac{\pi}{2(a_i + b_i)}} \left[\frac{1}{4(a_i + b_i)} \sqrt{\frac{\pi}{2(a_i + 2b_i)}} + \frac{\bar{r}_{1z}^2}{\bar{r}_{1x}^2 + \bar{r}_{1y}^2 + \bar{r}_{1z}^2} \sqrt{\frac{\pi}{2(a_i + 2b_i)}} \right] \\
&\quad + \sqrt{\frac{\pi}{2(a_i + 2b_i)}} \left(\frac{1}{4(a_i + b_i)} \bar{r}_{1y} \right) \\
&= 2 \left(\frac{\pi}{2(a_i + b_i)} \right)^{1/2} \left[\frac{1}{2(a_i + b_i)} + \bar{r}_{1z}^2 \right] e^{-2(a_i + b_i)\bar{r}_{1z}} \\
&= 2 \left(\frac{\pi}{2(a_i + b_i)} \right)^{3/2} \frac{3}{4(a_i + b_i)} \left[\frac{1}{2} + \frac{1}{4} \frac{\bar{r}_{1z}^2}{2 + \bar{r}_{1z}^2} \right]
\end{aligned}$$

③

$$\int \psi_2^* \psi_1 d^3 \vec{r} = \int \frac{(a_i + b_i)}{(d+i)^2} e^{-\frac{(d+i)^2}{(a_i+b_i)}} e^{-\frac{(r_1^2+r_2^2)}{(a_i+b_i)}} d^3 \vec{r}$$

$$= \frac{3}{4\sqrt{2}} \frac{\pi^{3/2}}{(a_i+b_i)^{5/2}}$$

Method 2

$$\text{Ansatz: } \left[\left(\frac{a_i + b_i}{d+i} \right)^{1/2} + P_{10} \right] e^{-(d+i)^2}$$

$$\text{Ansatz: } \left[\left(\frac{a_i + b_i}{d+i} \right)^{1/2} + \frac{c}{(d+i)^2} \right] \left(\frac{a_i + b_i}{d+i} \right)^{1/2}$$

$$\text{Ansatz: } \left[\frac{a_i + b_i}{(d+i)^2} + \frac{c}{(d+i)^3} + \frac{d}{(d+i)^4} \right] \left(\frac{a_i + b_i}{d+i} \right)^{1/2}$$

$$\text{Ansatz: } \left[\frac{a_i + b_i}{(d+i)^2} + P_{10} + \frac{c}{(d+i)^3} \right] \left(\frac{a_i + b_i}{d+i} \right)^{1/2}$$

$$\left[\frac{a_i + b_i}{(d+i)^2} + \frac{c}{(d+i)^3} + \frac{d}{(d+i)^4} \right] \left(\frac{a_i + b_i}{d+i} \right)^{1/2}$$

$$\text{Ansatz: } \left[\frac{a_i + b_i}{(d+i)^2} + P_{10} + \frac{c}{(d+i)^3} + \frac{d}{(d+i)^4} \right] \left(\frac{a_i + b_i}{d+i} \right)^{1/2}$$

$$\text{Ansatz: } \left[\frac{a_i + b_i}{(d+i)^2} + P_{10} + \frac{c}{(d+i)^3} + \frac{d}{(d+i)^4} \right] \left(\frac{a_i + b_i}{d+i} \right)^{1/2}$$

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Two Body Potential

$$\int \psi^* \nabla \psi d^3 \vec{r}_1 = \int (\psi_1^* \nabla \psi_1 + \psi_2^* \nabla \psi_2) d^3 \vec{r}_1$$

$$\begin{aligned} \int \psi_1^* \nabla \psi_1 &= \int d^3 \vec{r}_1 e^{-2(a_i + q_j) \vec{r}_1^2 - 4\lambda \vec{r}_1^2} \\ &= \int d^3 \vec{r}_1 e^{-(2a_i + 2q_j + 4\lambda) \vec{r}_1^2} \\ &= \left(\frac{\pi}{2a_i + 2q_j + 4\lambda} \right)^{3/2} \end{aligned}$$

$$\begin{aligned} \int \psi_2^* \nabla \psi_2 &= 4 \int d^3 \vec{r}_1 (\vec{r}_{1x}^2 + \vec{r}_{1y}^2 + \vec{r}_{1z}^2)^2 e^{-2(b_i + b_j) \vec{r}_1^2} e^{-4\lambda \vec{r}_1^2} \\ &= \frac{3}{\sqrt{2}} \frac{\pi^{3/2}}{(b_i + b_j + 2\lambda)^{7/2}} \end{aligned}$$

$$\begin{aligned} \int \psi_1^* \nabla \psi_2 &= 2 \int d^3 \vec{r}_1 (\vec{r}_{1x}^2 + \vec{r}_{1y}^2 + \vec{r}_{1z}^2) e^{-2(a_i + b_j) \vec{r}_1^2} e^{-4\lambda \vec{r}_1^2} \\ &= 2 \int d^3 \vec{r}_1 (\vec{r}_{1x}^2 + \vec{r}_{1y}^2 + \vec{r}_{1z}^2) e^{-2(a_i + b_j + 2\lambda) \vec{r}_1^2} \\ &= 2 \left[\frac{1}{4(a_i + b_j + 2\lambda)} + \vec{r}_{1y}^2 + \vec{r}_{1z}^2 \right] \left[\frac{\pi}{2a_i + 2b_j + 4\lambda} \right] \\ &\quad e^{-2(a_i + b_j + 2\lambda) \vec{r}_{1y}^2} e^{-2(a_i + b_j + 2\lambda) \vec{r}_{1z}^2} \end{aligned}$$

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$$\begin{aligned}
&= 2 \left(\frac{\pi}{2a_j + 2b_i + 4\lambda} \right)^{3/2} \left[\left[\frac{1}{4(a_j + b_i + 2\lambda)} + \frac{\pi^2}{4(a_j + b_i + 2\lambda)^2} \right] d\bar{\psi}_2 \right. \\
&\quad \left. + \frac{1}{2(a_j + b_i + 2\lambda)} \right] \\
&= 2 \left(\frac{\pi}{2a_j + 2b_i + 4\lambda} \right)^{3/2} \left[\frac{1}{2(a_j + b_i + 2\lambda)} + \frac{1}{4(a_j + b_i + 2\lambda)} \right] \\
&= 2 \left(\frac{\pi}{2a_j + 2b_i + 4\lambda} \right)^{3/2} \frac{3}{4(a_j + b_i + 2\lambda)} \\
&= \frac{3}{4\sqrt{2}} \left[\frac{\pi^{3/2}}{(a_j + b_i + 2\lambda)^{5/2}} \right] \frac{d}{(d+id)^{1/2}} \frac{d}{(d+id)^{1/2}} \\
\int \psi_2^* v \psi_1 &= \frac{3}{4\sqrt{2}} \left[\frac{\pi^{3/2}}{(a_j + b_i + 2\lambda)^{5/2}} \right] \frac{d}{(d+id)^{1/2}} \frac{d}{(d+id)^{1/2}} \\
&= \left[\frac{d}{(d+id)^{1/2}} \right]^2 \left(\frac{\pi}{a_j + b_i + 2\lambda} \right)^{3/2} = \frac{\pi^3}{8(a_j + b_i + 2\lambda)^3}
\end{aligned}$$

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Multiply $\frac{1}{2}$ factor in overall k.E.

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Kinetic Part :- $\Psi_1 = e^{-2a_i \bar{r}_1^2}$
 $\Psi_2 = 2\bar{r}_1^2 e^{-2b_i \bar{r}_1^2}$
 $\frac{\partial \Psi_1}{\partial \bar{r}_1} = -4a_i \bar{r}_1 e^{-2a_i \bar{r}_1^2}$
 $\frac{\partial \Psi_2}{\partial \bar{r}_1} = 2 \left[2\bar{r}_1 - 4b_i \bar{r}_1^3 \right] e^{-2b_i \bar{r}_1^2}$

$$\boxed{\Psi_2^* \frac{p^2}{2m} \Psi_2} = 16 (\bar{r}_1 - 2b_i \bar{r}_1^3) (\bar{r}_1 - 2b_i \bar{r}_1^3) e^{-2(b_i + b_j) \bar{r}_1^2}$$

$$= 16 (\bar{r}_1^2 - 2b_i \bar{r}_1^4 - 2b_i \bar{r}_1^4 + 4b_i b_j \bar{r}_1^6) e^{-2(b_i + b_j) \bar{r}_1^2}$$

$$= 16 (\bar{r}_1^2 - 2(b_i + b_j) \bar{r}_1^4 + 4b_i b_j \bar{r}_1^6) e^{-2(b_i + b_j) \bar{r}_1^2}$$

$$I_1 = \int \bar{r}_1^6 e^{-2(b_i + b_j) \bar{r}_1^2} e^{-2(b_i + b_j) \bar{r}_1^2} e^{-2(b_i + b_j) \bar{r}_1^2}$$

$$= \left[\frac{\pi}{2(b_i + b_j)} \right]^{3/2} \left[\frac{5!}{[4(b_i + b_j)]^3} + \frac{3(\bar{r}_{1y}^2 + \bar{r}_{1z}^2)}{[4(b_i + b_j)]^2} \right]^3$$

$$+ 3(\bar{r}_{1y}^4 + \bar{r}_{1z}^4) + 2\bar{r}_{1y}^2 \bar{r}_{1z}^2 \frac{1}{4(b_i + b_j)} + \bar{r}_{1y}^6 + \bar{r}_{1z}^6$$

$$+ 3\bar{r}_{1y}^4 \bar{r}_{1z}^2 + 3\bar{r}_{1z}^4 \bar{r}_{1y}^2$$

$$\begin{aligned}
& \left[\frac{\pi}{2(b_i+b_j)} \right]^{3/2} \left[\frac{5!}{[4(b_i+b_j)]^3} \right]^3 + \frac{3 \cdot 3!}{[4(b_i+b_j)]^2} \bar{\tau}_{12}^2 \\
& + \frac{3 \bar{\tau}_{12}^4}{4(b_i+b_j)} + \bar{\tau}_{12}^6 + \frac{1}{[4(b_i+b_j)]^2} \left[\frac{3 \cdot 3!}{[4(b_i+b_j)]^2} + \frac{6 \bar{\tau}_{12}^2}{4(b_i+b_j)} + 3 \bar{\tau}_{12}^4 \right] \\
& + \left[\frac{3}{4(b_i+b_j)} + \frac{3 \bar{\tau}_{12}^2}{4(b_i+b_j)} \right] \left[\frac{3!}{[4(b_i+b_j)]^2} + \frac{5!}{[4(b_i+b_j)]^3} \right] \\
\Rightarrow & \left[\frac{\pi}{2(b_i+b_j)} \right]^{3/2} \left[\frac{5!}{64(b_i+b_j)^3} + \frac{3 \cdot 3!}{64(b_i+b_j)^3} \right. \\
& + \frac{3 \cdot 3!}{64(b_i+b_j)^3} + \frac{5!}{64(b_i+b_j)^3} + \frac{3 \cdot 3!}{64(b_i+b_j)^3} \\
& + \frac{6}{64(b_i+b_j)^3} + \frac{3 \cdot 3!}{64(b_i+b_j)^3} + \frac{3 \cdot 3!}{64(b_i+b_j)^3} \\
& + \left. \frac{3 \cdot 3!}{64(b_i+b_j)^3} + \frac{5!}{64(b_i+b_j)^3} \right] \\
= & \left[\frac{\pi}{2(b_i+b_j)} \right]^{3/2} \left[120 + 18 + 18 + 120 + 18 + 6 + 18 + 18 + 18 + 120 \right] \frac{1}{64(b_i+b_j)^3} \\
\Rightarrow & \frac{\pi^{3/2}}{(b_i+b_j)^{9/2}} \frac{474}{128\sqrt{2}} = \frac{2.61 \pi^{3/2}}{(b_i+b_j)^{9/2}}
\end{aligned}$$

$$\cancel{\frac{1}{I_2}} = \int \bar{x}_1^4 e^{-2(b_i + b_j) \frac{\bar{x}_1^2}{\bar{x}_1^2}}$$

$$= \int (\bar{x}_{1x}^4 + \bar{x}_{1y}^4 + \bar{x}_{1z}^4 + 2\bar{x}_{1x}^2 \bar{x}_{1y}^2 + 2\bar{x}_{1y}^2 \bar{x}_{1z}^2 + 2\bar{x}_{1z}^2 \bar{x}_{1x}^2) e^{-2(b_i + b_j) \bar{x}_1^2}$$

$$= \left[\frac{\pi}{2(b_i + b_j)} \right]^{3/2} \left[\frac{3!}{[4(b_i + b_j)]^2} + \frac{2(\bar{x}_{1y}^2 + \bar{x}_{1z}^2)}{84(b_i + b_j)} + \bar{x}_{1y}^4 + \bar{x}_{1z}^4 + 2\bar{x}_{1y}^2 \bar{x}_{1z}^2 \right]$$

$$= \left[\frac{\pi}{2(b_i + b_j)} \right]^{3/2} \left[\frac{3!}{[4(b_i + b_j)]^2} + \frac{2\bar{x}_{1z}^2}{4(b_i + b_j)} + \bar{x}_{1z}^4 + \left(\frac{2}{4(b_i + b_j)} + 2\bar{x}_{1z}^2 \right) \frac{1}{4(b_i + b_j)} + \frac{3!}{[4(b_i + b_j)]^2} \right]$$

$$= \left[\frac{\pi}{2(b_i + b_j)} \right]^{3/2} \left[\frac{3!}{[4(b_i + b_j)]^2} + \frac{2}{[4(b_i + b_j)]^2} + \frac{3!}{[4(b_i + b_j)]^2} \right]$$

$$+ \frac{2}{[4(b_i + b_j)]^2} + \frac{2}{[4(b_i + b_j)]^2} + \frac{3!}{[4(b_i + b_j)]^2}$$

$$= \left[\frac{\pi}{2(b_i + b_j)} \right]^{3/2} \left[\frac{24^3}{16(b_i + b_j)^2} \right] = \frac{3}{4\sqrt{2}} \frac{\pi^{3/2}}{(b_i + b_j)^{7/2}}$$

$$I_3 = \int (\bar{r}_{1x}^2 + \bar{r}_{1y}^2 + \bar{r}_{1z}^2) e^{-2(b_i + b_j)\bar{r}_1^2} d^3\bar{r}_1$$

$$= \left[\frac{\pi}{2(b_i + b_j)} \right]^{3/2} \left[\frac{3}{4(b_i + b_j)} \right]$$

$$= \frac{3 \pi^{3/2}}{8\sqrt{2} (b_i + b_j)^{5/2}}$$

~~Q0,~~

$$\Psi_2^* \frac{p^2}{2m} \Psi_2 = 16 \left[\frac{3 \pi^{3/2}}{8\sqrt{2} (b_i + b_j)^{5/2}} - \frac{4(b_i + b_j) 3 \pi^{3/2}}{4\sqrt{2} (b_i + b_j)^{7/2}} + \frac{16 b_i b_j 2.61 \pi^{3/2}}{(b_i + b_j)^{9/2}} \right]$$

$$= 16 \left[\frac{3 \pi^{3/2}}{8\sqrt{2} (b_i + b_j)^{5/2}} - \frac{3 \pi^{3/2}}{\sqrt{2} (b_i + b_j)^{5/2}} + \frac{41.76 b_i b_j \pi^{3/2}}{(b_i + b_j)^{9/2}} \right]$$

$$= 16 \left[\frac{3 \pi^{3/2}}{\sqrt{2} (b_i + b_j)^{5/2}} \left(-\frac{7}{8} \right) + \frac{41.76 b_i b_j \pi^{3/2}}{(b_i + b_j)^{9/2}} \right]$$

$$= \frac{\pi^{3/2}}{(b_i + b_j)^{5/2}} \left[-\frac{21x+6}{8\sqrt{2}} + \frac{41.76 b_i b_j}{(b_i + b_j)^{4/2}} \right]$$

$$\frac{1}{8} - 1 \Rightarrow -\frac{7}{8}$$

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Total k.E

$$\begin{aligned}
 & 16 \left[\frac{4 b_i b_j 2.61 \pi^{3/2}}{(b_i + b_j)^{9/2}} - \frac{2(b_i + b_j)^3 \pi^{3/2}}{4\sqrt{2} (b_i + b_j)^{7/2}} \right. \\
 & \quad \left. + \frac{3}{8\sqrt{2}} \frac{\pi^{3/2}}{(b_i + b_j)^{5/2}} \right] \\
 & 16 \left[\frac{2.61 \times 4 b_i b_j \pi^{3/2}}{(b_i + b_j)^{9/2}} - \frac{6 \pi^{3/2}}{4\sqrt{2} (b_i + b_j)^{5/2}} + \frac{3 \pi^{3/2}}{8\sqrt{2} (b_i + b_j)^{5/2}} \right] \\
 = & 16 \left[\frac{2.61 \times 4 b_i b_j}{(b_i + b_j)^2} - \frac{3}{2\sqrt{2}} + \frac{3}{8\sqrt{2}} \right] \frac{\pi^{3/2}}{(b_i + b_j)^{5/2}} \\
 = & 16 \left[\frac{2.61 \times 4 b_i b_j}{(b_i + b_j)^2} - \frac{9}{8\sqrt{2}} \right] \frac{\pi^{3/2}}{(b_i + b_j)^{5/2}} \\
 = & \frac{\pi^{3/2}}{(b_i + b_j)^{5/2}} \left[\frac{64 \times 2.61 b_i b_j}{(b_i + b_j)^2} - \frac{18}{\sqrt{2}} \right] \\
 = & \frac{2 \pi^{3/2}}{(b_i + b_j)^{5/2}} \left[\frac{2.61 \times 32 b_i b_j}{(b_i + b_j)^2} - \frac{9}{\sqrt{2}} \right] = \psi_2^* \frac{p^2}{2m} \psi_2
 \end{aligned}$$

$$\begin{aligned}
\Psi_1^* \frac{p_i^2}{2m} \Psi_2 &= -16 a_i \bar{\pi}_i^2 (\bar{\pi}_i - 2b_i \bar{\pi}_i^2) e^{-2(a_i + b_i) \bar{\pi}_i^2} \\
&= -16 a_i \left[\bar{\pi}_i^2 - 2b_i \bar{\pi}_i^4 \right] e^{-2(a_i + b_i) \bar{\pi}_i^2} \\
&= -16 a_i \left[\frac{3 \pi^{3/2}}{8\sqrt{2} (a_i + b_i)^{5/2}} - \frac{2b_i 3 \pi^{3/2}}{4\sqrt{2} (a_i + b_i)^{7/2}} \right] \\
&= \frac{-16 a_i \pi^{3/2}}{(a_i + b_i)^{5/2}} \left[\frac{3}{8\sqrt{2}} - \frac{6b_i}{24\sqrt{2} (a_i + b_i)} \right] \\
&= \frac{-16 a_i \pi^{3/2}}{(a_i + b_i)^{5/2}} \frac{3}{2\sqrt{2}} \left[\frac{1}{4} - \frac{b_i}{(a_i + b_i)} \right] \\
&= \cancel{\frac{-16 a_i \pi^{3/2}}{2\sqrt{2} (b_i + b_i)^{5/2}} \left[\frac{b_i - 3b_i}{4(b_i + b_i)} \right]} \quad b_i + b_i - 4b_i \\
&= \cancel{\frac{3\sqrt{2} a_i \pi^{3/2}}{(b_i + b_i)^{7/2}} \left[\frac{b_i - 3b_i}{4(b_i + b_i)} \right]} \quad a_i + b_i - 4b_i \\
&= \frac{-8 a_i \pi^{3/2} 3}{\sqrt{2} (a_i + b_i)^{5/2}} \left[\frac{a_i - 3b_i}{4(a_i + b_i)} \right]
\end{aligned}$$

$$\Psi_1 \frac{b^2}{8m} \Psi_1 = b$$

$$= 16 q_i q_j \bar{r}_1^2 e^{-2(q_i + q_j) \bar{r}_1^2}$$

$$= \frac{16 q_i q_j \pi^{3/2}}{8\sqrt{2} (q_i + q_j)^{5/2}}$$

$$= \frac{3\sqrt{2} q_i q_j \pi^{3/2}}{(q_i + q_j)^{5/2}}$$

Summary

Indian Institute of Technology Guwahati

(Supplementary Answer Sheet)

Name of Student :		Roll No.
Course No.		Signature of the student :

$$\Psi = \sum_{i=1}^N c_i e^{-a_i(\bar{r}_1^2 + \bar{r}_2^2)} + \sum_{j=N+1}^{\infty} d_j (\bar{r}_1^2 + \bar{r}_2^2) e^{-b_j(\bar{r}_1^2 + \bar{r}_2^2)}$$

$$\Psi = \Psi_1 + \Psi_2 \Rightarrow b_1 \Psi_1 = \sum_{i=1}^N c_i e^{-a_i(\bar{r}_1^2 + \bar{r}_2^2)}$$

$$\Psi_2 = \sum_{j=N+1}^{\infty} d_j (\bar{r}_1^2 + \bar{r}_2^2) e^{-b_j(\bar{r}_1^2 + \bar{r}_2^2)}$$

Norm $\int \Psi^* \Psi d\tau$

$$\int (\Psi_1 + \Psi_2)^* (\Psi_1 + \Psi_2) d\tau = \int (\Psi_1^* \Psi_1 + \Psi_1^* \Psi_2 + \Psi_2^* \Psi_1 + \Psi_2^* \Psi_2) d\tau$$

$$\Psi_1^* = \sum_{k=1}^N c_k e^{-a_k(\bar{r}_1^2 + \bar{r}_2^2)}$$

$$\Psi_2^* = \sum_{l=N+1}^{\infty} d_l (\bar{r}_1^2 + \bar{r}_2^2) e^{-b_l(\bar{r}_1^2 + \bar{r}_2^2)}$$

$$\Psi_1^* \Psi_1 = \left[\frac{\pi}{2(b_1 + b_2)} \right]^{3/2}$$

$$\Psi_2^* \Psi_2 = \frac{3}{\sqrt{2}} \frac{\pi^{3/2}}{(c_1 + c_2)^{7/2}}$$

$$\Psi_1^* \Psi_2 = \frac{3}{4\sqrt{2}} \frac{\pi^{3/2}}{(b_1 + b_2)^{5/2}}$$

$$\Psi_2^* \Psi_1 = \frac{3}{4\sqrt{2}} \frac{\pi^{3/2}}{(c_1 + b_2)^{5/2}}$$

$$b_1 = k \\ b_2 = l \quad] \text{ widths } \square$$

$$c_1 = l \\ c_2 = j \quad] \text{ widths } \square$$

Two body potential $\langle \Psi | V_2 | \Psi \rangle$

$$V_2 = C_0 e^{-\lambda(\bar{r}_1 - \bar{r}_2)^2} = C_0 e^{-4\lambda \bar{r}_1^2}$$

$$I = \int \Psi_1^* V_2 \Psi_1 + \int \Psi_2^* V_2 \Psi_2 + \int \Psi_1^* V_2 \Psi_2 \\ + \int \Psi_2^* V_2 \Psi_1$$

$$\Psi_1^* V_2 \Psi_1 = \frac{\pi^{3/2}}{(2b_1 + 2b_2 + \lambda^2)^{3/2}}$$

$$\begin{aligned} b_2 &= i \\ b_1 &= k \\ c_1 &= l \\ c_2 &= j \end{aligned}$$

$$\Psi_2^* V_2 \Psi_2 = \frac{3}{\sqrt{2}} \frac{\pi^{3/2}}{(c_1 + c_2 + 0.5\lambda^2)^{7/2}}$$

$$\Psi_1^* V_2 \Psi_2 = \frac{3}{4\sqrt{2}} \frac{\pi^{3/2}}{(b_1 + c_2 + \frac{\lambda^2}{2})^{5/2}}$$

$$\Psi_2^* V_2 \Psi_1 = \frac{3}{4\sqrt{2}} \frac{\pi^{3/2}}{(c_1 + b_2 + \frac{\lambda^2}{2})^{5/2}}$$

$$\begin{aligned} \Psi_1 &= b_2 \\ \Psi_1^* &= b_1 \\ \Psi_2 &= c_2 \\ \Psi_2^* &= c_1 \end{aligned}$$

Kinetic Part

$$\psi_1^* \frac{p^2}{2m} \psi_1 = -\frac{3 b_1 b_2 \pi^{3/2}}{\sqrt{2} (b_1 + b_2)^{5/2}}$$

$$\psi_2^* \frac{p^2}{2m} \psi_2 = 4 \sqrt{\frac{\pi}{2c_1 + 2c_2}} \left(\frac{-5}{4c_1 + 4c_2} + \frac{30 c_1 c_2}{(c_1 + c_2)^3} \right)$$

~~$$\psi_1^* \frac{p^2}{2m} \psi_2 = \frac{3\sqrt{2} b_1 \pi^{3/2}}{(b_1 + c_2)^{7/2}} (b_1 - 3c_2)$$~~

~~$$\psi_2^* \frac{p^2}{2m} \psi_1 = \frac{3\sqrt{2} b_2 \pi^{3/2}}{(b_2 + c_1)^{7/2}} (b_2 - 3c_1)$$~~

Kinetic Part

$$\psi_1^* \frac{p^2}{2m} \psi_1 = -\frac{3 b_1 b_2 \pi^{3/2}}{\sqrt{2} (b_1 + b_2)^{5/2}}$$

$$\psi_2^* \frac{p^2}{2m} \psi_2 = \frac{\pi^{3/2}}{(B_1 + B_2)^{5/2}} \left[\frac{83.52 B_1 C_2}{(B_1 + B_2)^2} - \frac{9}{\sqrt{2}} \right]$$

$$\psi_1^* \frac{p^2}{2m} \psi_2 = -\frac{3}{\sqrt{2}} \frac{b_1 \pi^{3/2}}{(b_1 + c_2)^{7/2}} (b_1 - 3c_2)$$

$$\psi_2^* \frac{p^2}{2m} \psi_1 = -\frac{3}{\sqrt{2}} \frac{b_2 \pi^{3/2}}{(b_2 + c_1)^{7/2}} (b_2 - 3c_1)$$