Indian Institute of Technology Guwahati

(Supplementary Answer Sheet)

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

$$\phi_2 = 2\left(\bar{r}_1^2 + \bar{r}_2^2 + \bar{r}_1\bar{r}_2\right) e^{-2b_1\left(\bar{r}_1^2 + \bar{r}_2^2 + \bar{r}_1\bar{r}_2\right)}$$

$$\phi_2^* \phi_2 = 4\left(\bar{r}_1^2 + \bar{r}_2^2 + \bar{r}_1\bar{r}_2\right)^2 e^{-2(b_1+b_2)\left(\bar{r}_1^2 + \bar{r}_2^2 + \bar{r}_1\bar{r}_2\right)}$$

$$= 4\left(\underline{\bar{r}_1^4 + \bar{r}_2^4} + 2\bar{r}_1^2\bar{r}_2^2 + \bar{r}_1^2 \cdot \bar{r}_2^2 + 2\bar{r}_1^2(\bar{r}_1\bar{r}_2) + 2\bar{r}_2^2(\bar{r}_1\bar{r}_2)\right) e^{-2(b_1+b_2)\left(\bar{r}_1^2 + \bar{r}_2^2 + \bar{r}_1\bar{r}_2\right)}$$

$$= 4\left[\frac{2}{3(a+b)^2} + \frac{3}{6(a+b)^2} \cancel{+} \frac{2}{6(a+b)^2} - \frac{2}{6(a+b)^2}\right]$$

$$= \frac{2}{(a+b)^2} \frac{(2\pi)^3 \quad 3}{12\sqrt{12}\ (a+b)^3}$$

$$= \frac{2 \times \cancel{8} \times \cancel{3}\ \pi^3}{\cancel{24}\sqrt{3}\ (a+b)^5} = \frac{2\pi^3}{\sqrt{3}\ (a+b)^5}$$

Some Important Integrations

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$$I_1 = \int \bar{r}_1^4 \, e^{-2(b_1+b_2)(\bar{r}_1^2+\bar{r}_2^2+\bar{r}_1\bar{r}_2)}$$

$$\int \bar{r}_1 \bar{r}_2 \bar{r}_3 \bar{r}_4 \, e^{-\frac{1}{2}V^T A V} dV = \int \bar{r}_1 \bar{r}_1 \bar{r}_1 \bar{r}_1 \, e^{-\frac{1}{2}V^T A V} dV$$

$$= 3 A^{-1}_{11} A^{-1}_{11}$$

$$\boxed{I_1 = 3 \frac{1}{(3a+3b)^2} = \frac{1}{3(a+b)^2}}$$

$$I_2 = \int \bar{r}_1^2 \bar{r}_2^2 \, e^{-2(b_1+b_2)(\bar{r}_1^2+\bar{r}_2^2+\bar{r}_1\bar{r}_2)} d^3\bar{r}_1 \, d^3\bar{r}_2$$

$$= A^{-1}_{11} A^{-1}_{22} + A^{-1}_{12} A^{-1}_{12} + A^{-1}_{12} A^{-1}_{12}$$

$1 \to 1$
$2 \to 1$
$3 \to 2$
$4 \to 2$

$$= \frac{1}{9(a+b)^2} + \frac{1}{36(a+b)^2} + \frac{1}{36(a+b)^2}$$

$$\boxed{I_2 = \frac{1}{6(a+b)^2}}$$

$$I_3 = \int \bar{r}_1^3 \bar{r}_2 \, e^{-2(b_1+b_2)(\bar{r}_1^2+\bar{r}_2^2+\bar{r}_1\bar{r}_2)} d^3\bar{r}_1 \, d^3\bar{r}_2$$

$1 \to 1$
$2 \to 1$
$3 \to 1$
$4 \to 2$

$$A^{-1}_{11} A^{-1}_{12} + A^{-1}_{11} A^{-1}_{12} + A^{-1}_{12} A^{-1}_{11}$$

$$= 3 \left(\frac{1}{3a+3b} \right) \left(-\frac{1}{6a+6b} \right) = -\frac{1}{6(a+b)^2}$$

$$\boxed{I_3 = -\frac{1}{6(a+b)^2}}$$

$$I_4 = \int \bar{r}_1 \bar{r}_2^3 \, e^{-2(b_1+b_2)(\bar{r}_1^2+\bar{r}_2^2+\bar{r}_1\bar{r}_2)}$$

$$= A^{-1}_{12} A^{-1}_{22} + A^{-1}_{12} A^{-1}_{22} + A^{-1}_{12} A^{-1}_{22}$$

$$= 3\left(\frac{1}{3a+3b}\right)\left(-\frac{1}{6a+6b}\right) = -\frac{1}{6(a+b)^2}$$

$$\boxed{I_4 = -\frac{1}{6(a+b)^2}}$$

<u>Multiply by</u> $\left[\frac{(2\pi)}{\sqrt{A}}\right]^3 = \frac{8\pi^3}{(A)^{3/2}}$

$$|A| = 12(a+b)^2$$

$$A^{-1} = \begin{pmatrix} \frac{1}{3a+3b} & -\frac{1}{6a+6b} \\ -\frac{1}{6a+6b} & \frac{1}{3a+3b} \end{pmatrix}$$