Solution 7

1. (a) Consider the $d^3\mathbf{r}_1$ in spherical coordinates, and the $d^3\mathbf{r}_2$ in cylindrical coordinates. Align $\mathbf{r}_2$'s cylindrical coordinate system along $\mathbf{r}_1$ so the cylindrical coordinate z becomes $r_{||}$ and the cylindrical coordinate r becomes $r_\perp$, leaving only the cylindrical coordinate ϕ.

   So:

$$d^3\mathbf{r}_1\, d^3\mathbf{r}_2 \,=(r_1^2 Sin\theta_1 dr_1 d\theta_1 d\phi_1)(r_\perp dr_\perp d\phi_2 dr_{||})$$

   and since the expectation value integrals have no explicit angle dependence, we can integrate away all the angles, giving

$$d^3\mathbf{r}_1\, d^3\mathbf{r}_2 \,=(4\pi r_1^2 dr_1)(2\pi r_\perp dr_\perp dr_{||})$$

   (b) From the picture on page 2, it is clear:

$$r_2 = \sqrt{r_{||}^2 + r_\perp^2}$$
$$r_{12} = |\mathbf{r}_1 - \mathbf{r}_2| = |\mathbf{r}_1 - \mathbf{r}_{||} - \mathbf{r}_\perp| = |\hat{r}_1(|r_1| - |r_{||}|) - \hat{r}_\perp |r_\perp|| = \sqrt{r_1^2 + r_{||}^2 - 2r_1 r_{||} + r_\perp^2}$$
$$r_1 = r_1$$

   With these formulas for the lengths of $\{r_2,\, r_{12},\, r_1\}$ in terms of the lengths $\{r_{||},\, r_\perp,\, r_1\}$ we can now compute the Jacobian.

$$J = \begin{vmatrix} \frac{\partial r_2}{\partial r_{||}} & \frac{\partial r_2}{\partial r_\perp} & \frac{\partial r_2}{\partial r_1} \\ \frac{\partial r_{12}}{\partial r_{||}} & \frac{\partial r_{12}}{\partial r_\perp} & \frac{\partial r_{12}}{\partial r_1} \\ \frac{\partial r_1}{\partial r_{||}} & \frac{\partial r_1}{\partial r_\perp} & \frac{\partial r_1}{\partial r_1} \end{vmatrix} = \begin{vmatrix} \frac{r_{||}}{r_2} & \frac{r_\perp}{r_2} & 0 \\ \frac{r_{||}-r_1}{r_{12}} & \frac{r_\perp}{r_{12}} & \frac{r_1 - r_{||}}{r_{12}} \\ 0 & 0 & 1 \end{vmatrix} = \frac{r_1 r_\perp}{r_2 r_{12}}$$

   And so

$$r_2 r_{12} dr_1 dr_2 dr_{12} = r_1 r_\perp dr_1 dr_\perp dr_{||} \quad .$$

   Now, remember r_{12} is the length of a vector, and as such, it cannot be negative. Also, from the definition of r_{12}, it is clear it cannot be greater than $r_1 + r_2$. If you consider all different r_1 and r_2 lengths, they can be broken into two regimes. One where $r_1 > r_2$ (in which case $\min r_{12} = r_1 - r_2$) and the other where $r_2 > r_1$ (in which case $\min r_{12} = r_2 - r_1$).

   And so

$$\int_{all\, r_1,\, r_2} = \int_0^\infty dr_1 \int_{r_1}^\infty dr_2 \int_{r_2 - r_1}^{r_2 + r_1} dr_{12} + \int_0^\infty dr_2 \int_{r_2}^\infty dr_1 \int_{r_1 - r_2}^{r_1 + r_2} dr_{12}$$

But since the function is symmetric with respect to interchanging 1 and 2, these last 2 integrals are really the same. So,

$$\int d^3\mathbf{r}_1\, d^3\mathbf{r}_2\, f(\cdots) =$$

$$8\pi^2 \int_0^\infty r_1^2\, dr_1 \int_0^\infty r_\perp\, dr_\perp \int_0^\infty dr_{||}\, f(\cdots) =$$

$$16\pi^2 \int_0^\infty r_1\, dr_1 \int_{r_1}^\infty r_2\, dr_2 \int_{r_2-r_1}^{r_2+r_1} r_{12}\, dr_{12}\, f(\cdots)$$

(c) First note $\{r_{12},\, r_1,\, r_2\}$ is convenient shorthand for

$$\begin{aligned} r_{12} &= \sqrt{(x_1-x_2)^2+(y_1-y_2)^2+(z_1-z_2)^2} \\ r_1 &= \sqrt{x_1^2+y_1^2+z_1^2} \\ r_2 &= \sqrt{x_2^2+y_2^2+z_2^2} \end{aligned}$$

Which imply

$$\vec{\nabla}_1\, |\vec{\mathbf{r}}_1| = \tfrac{\vec{\mathbf{r}}_1}{r_1} \qquad \vec{\nabla}_1\, |\vec{\mathbf{r}}_1 - \vec{\mathbf{r}}_2| = \tfrac{\vec{\mathbf{r}}_1-\vec{\mathbf{r}}_2}{r_{12}}$$

$$\nabla_1^2\, |\vec{\mathbf{r}}_1| = \tfrac{1}{r_1}\, \left(\tfrac{\partial}{\partial r_1}\right)^2 r_1^2 = \tfrac{2}{r_1} \qquad \nabla_1^2\, |\vec{\mathbf{r}}_{12}| = \tfrac{2}{r_{12}}$$

with this in mind,

$$\begin{aligned} &\nabla_1^2\,(1+W\,r_{12})\; e^{-Z\,(r_1+r_2)} = \vec{\nabla}_1\cdot\vec{\nabla}_1\,(1+W\,r_{12})\; e^{-Z\,(r_1+r_2)} \\ &= \vec{\nabla}_1\cdot\left(W\,\vec{\nabla}_1 r_{12}\, e^{-Z\,(r_1+r_2)} + (1+W\,r_{12})\,\vec{\nabla}_1\, e^{-Z\,(r_1+r_2)}\right) \\ &= W\;(\nabla_1^2 r_{12})\; e^{-Z\,(r_1+r_2)} + 2\,W\;\left(\vec{\nabla}_1 r_{12}\right)\cdot\left(\vec{\nabla}_1\, e^{-Z\,(r_1+r_2)}\right) + (1+W\,r_{12})\,\left(\nabla_1^2\, e^{-Z\,(r_1+r_2)}\right) \\ &= W\,\tfrac{2}{r_{12}}\, e^{-Z\,(r_1+r_2)} + 2\,W\,\tfrac{\vec{\mathbf{r}}_1-\vec{\mathbf{r}}_2}{r_{12}}\cdot\left(e^{-Z\,(r_1+r_2)}(-Z\tfrac{\vec{\mathbf{r}}_1}{r_1})\right) + \\ &(1+W\,r_{12})\left(e^{-Z\,(r_1+r_2)}\left(\tfrac{-Z\,\vec{\mathbf{r}}_1}{r_1}\right)\cdot\left(\tfrac{-Z\,\vec{\mathbf{r}}_1}{r_1}\right) + \; e^{-Z\,(r_1+r_2)}(-Z\,\tfrac{2}{r_1})\right) \\ &= e^{-Z\,(r_1+r_2)}\left(\tfrac{2W}{r_{12}} - \tfrac{2\,Z\,W\,(r_1^2-\vec{\mathbf{r}}_1\cdot\vec{\mathbf{r}}_2)}{r_1 r_{12}} + (1+W\,r_{12})\left(Z^2-\tfrac{2\,Z}{r_1}\right)\right) \end{aligned}$$

Now note $r_1^2 - r_2^2 + r_{12}^2 = 2\,r_1^2 - 2\,\vec{\mathbf{r}}_1\cdot\vec{\mathbf{r}}_2$ and so this simplifies to,

$$\nabla_1^2\psi = e^{-Z\,(r_1+r_2)} \quad \times$$

$$\left(\frac{2W}{r_{12}} - \frac{ZW}{r_{12}}\frac{r_1^2-r_2^2+r_{12}^2}{r_1} + (1+W\,r_{12})(Z^2-\frac{2Z}{r_1})\right) \quad .$$

Thus,

$$\frac{-1}{2}\nabla_1^2\psi + \frac{-1}{2}\nabla_2^2\psi = e^{-Z\,(r_1+r_2)} \quad \times$$

$$\left(\frac{-2W}{r_{12}} + \frac{ZW}{2r_{12}}\left(\frac{r_1^2 - r_2^2 + r_{12}^2}{r_1} + \frac{r_2^2 - r_1^2 + r_{12}^2}{r_2}\right) + (1 + W\, r_{12})\left(\frac{Z}{r_1} + \frac{Z}{r_2} - Z^2\right)\right) \quad .$$

(d) Nothing to show...

(e)

$$\frac{\partial E(Z,0)}{\partial Z} = 2Z - \frac{22}{16} = 0 \quad \Rightarrow z = \frac{11}{16}$$

This corresponds to an energy of $-\frac{121}{256} = -.472656$, just above $-\frac{1}{2}$.

(f) Minimum is reached at $Z = .825726$ and $W = .493351$, which makes an energy of $E = -.50878$.

(e) AWE!