Hints on integrals in Midterm Problem 3

I was told repeatedly by Ed that you are having difficulties with some of the integrals in Problem 3 in the take-home midterm. There are many ways to do the integrals, but here are some of them.

(1) Numerical. You can always resort to numerical integration. Trick is to perform angular integrals as much as possible, and do the radial integrals numerically. Z' dependence can be factored out by changing the integration variable from r_i ($i = 1, 2$) to $\rho_i = Z'r_1/a_0$. If you use Mathematica, it can probably estimate the integral from 0 to ∞. If you write your own code, make sure that you change your integration variable to make the integration region finite; for instance using $z = e^{-\rho}$ or $e^{-2\rho}$ as the variable makes the integration range $[0, \infty)$ to $[0, 1]$ and can make the integrand more or less flat thanks to the Jacobian. Convergence is much faster this way and the result is more trustworthy. You may find logarithmic singularities, which you can deal with by subtracting logs which can be analytically integrated.

(2) Analytical. I imagine the difficulty you are having is the integral with powers of r_{12}. When the power is even, $r_{12}^2 = r_1^2 + r_2^2 - 2r_1r_2\cos\theta_{12}$ allows you to perform angular integrations first, and then the rest is just integrals over r_1 and r_2 which Mathematica can do. When the power is odd, you can use the formula we used before

$$\begin{aligned} \frac{1}{r_{12}} &= \sum_{l=0}^{\infty} \frac{r_<^l}{r_>^{l+1}} P_l(\cos\theta_{12}), \\ P_l(\cos\theta_{12}) &= \frac{4\pi}{2l+1} \sum_{m=-l}^{l} Y_l^{m*}(\theta_1, \phi_1) Y_l^m(\theta_2, \phi_2). \end{aligned} \tag{1}$$

In case you are curious, the first formula is the immediate consequence of the generating function for Legendre polynomials

$$\frac{1}{\sqrt{1 - 2tu + t^2}} = \sum_{l=0}^{\infty} t^l P_l(u) \qquad (|t| < 1), \tag{2}$$

where $u = \cos\theta_{12}$, $t = r_</r_>$ and $\sqrt{1 - 2tu + t^2} = r_{12}/r_>$.

When you have, say, r_{12} instead of $1/r_{12}$, you can expand it as

$$\begin{aligned} r_{12} &= r_{12}^2 \frac{1}{r_{12}} \\ &= (r_1^2 + r_2^2 - 2r_1r_2\cos\theta_{12}) \sum_{l=0}^{\infty} \frac{r_<^l}{r_>^{l+1}} P_l(\cos\theta_{12}). \end{aligned} \tag{3}$$

Now you can use recursion relation of the Legendre polynomials

$$nP_n(x) - (2n-1)xP_{n-1}(x) + (n-1)P_{n-2}(x) = 0. \tag{4}$$

In case this doens't ring the bell, I can rewrite it as

$$xP_n(x) = \frac{n+1}{2n+1}P_{n+1}(x) + \frac{n}{2n+1}P_{n-1}(x). \tag{5}$$

This is basically the addition of two angular momenta, $l = 1$ ($P_1(x) = x$) and l to $l+1$ and $l-1$. Using this recursion relation, $\cos\theta_{12} P_l(\cos\theta_{12})$ can be rewritten in terms of $P_{l\pm 1}(\cos\theta_{12})$. You can further change the index l to $l \pm 1$ and find

$$r_{12} = \sum_{l=0}^{\infty} \frac{r_<^l}{r_>^{l+1}} \left(\frac{r_<^2}{2l+3} - \frac{r_>^2}{2l-1} \right) P_l(\cos\theta_{12}) \tag{6}$$

To obtain general formulae for odd powers of r_{12}, here is a way to systematically derive them. There are formulae to expand a spherical waves in terms of spherical Bessel functions,

$$\frac{\sin kr_{12}}{r_{12}} = k\sum_{l=0}^{\infty}(2l+1)j_l(kr_1)j_l(kr_2)P_l(\cos\theta_{12}), \tag{7}$$

$$\frac{\cos kr_{12}}{r_{12}} = k\sum_{l=0}^{\infty}(2l+1)j_l(kr_<)n_l(kr_>)P_l(\cos\theta_{12}). \tag{8}$$

Together with this, you need the power series expansion of spherical Bessel functions (in Messiah's sign convention for n_n),

$$j_n(z) = (2z)^n \sum_{m=0}^{\infty} \frac{(-1)^m (n+m)!}{m!(2n+2m+1)!} z^{2m}, \tag{9}$$

$$n_n(z) = \frac{1}{2^n z^{n+1}} \sum_{m=0}^{\infty} \frac{\Gamma(2n-2m+1)}{m!\Gamma(n-m+1)} z^{2m}. \tag{10}$$

The formula Eq. (1) is obtained from Eq. (8) by taking the limit $k \to 0$. But you can also take $O(k^2)$ terms to obtain the expansion of r_{12} in Eq. (6) and similarly higher powers $O(k^{2n})$ to obtain the expansion of r_{12}^{2n-1} in terms of Legendre polynomials.

I hope this set of hints helps.