$$\langle \tfrac{1}{r} \rangle_{ij} = \int_{-\infty}^{\infty} dt \left[\int_{-\infty}^{\infty} (x-x_i)^m (x-x_j)^n e^{-bx^2} e^{-x^2t^2} dx \int dy \int dz \right]$$

其中 正

$$\int_{-\infty}^{\infty} (x-x_i)^m (x-x_j)^n e^{-(b+t^2)x^2} dx. \qquad \int_{-\infty}^{\infty} e^{-(b+t^2)x^2} dx = \sqrt{\frac{\pi}{b+t^2}}$$

$$\int_{-\infty}^{\infty} (y-y_i)^m (y-y_j)^n e^{-(b+t^2)y^2} dy$$

$$\int_{-\infty}^{\infty} (z-z_i)^m (z-z_j)^n e^{-b(z-R)^2 - t^2z^2} dz.$$

$$e^{-b(z-R)^2} \cdot e^{-t^2z^2} = e^{-b\frac{R^2t^2}{t^2+b}} e^{-(b+t^2)\cdot\left(z - \frac{R\overset{b}{\cancel{t^2}}}{t^2+b}\right)^2}$$

$\Downarrow$ 最后积出 dt:

x, y, z 积出来的

$$\sum_m \int_{-\infty}^{\infty} coe \cdot (t^2+b)^{-\frac{m}{2}} e^{-b\frac{R^2t^2}{t^2+b}} dt, \quad m = 3、5、7\cdots$$

$$\xrightarrow[t^2 = \frac{bu^2}{1-u^2}]{\frac{t^2}{t^2+b} = u^2} 2\sum_m \int_0^1 coe \left(\frac{bu^2}{1-u^2} + \frac{b-bu^2}{1-u^2} \right)^{-\frac{m}{2}} e^{-bR^2u^2} \sqrt{b}\, (1-u^2)^{-\frac{3}{2}} du$$

$$= 2\sum_m b^{\frac{1-m}{2}} \int_0^1 coe (1-u^2)^{\frac{m}{2}-\frac{3}{2}} e^{-bR^2u^2} du$$

$$= 2\sum_m (-1)^k b^{-(k+1)} coe(2k+3) \int_0^1 (u-1)^k (u+1)^k e^{-bR^2u^2} du \qquad k = \frac{m-3}{2} = 0, 1, 2\cdots$$

$$\int_0^1 x^n e^{-bx^2}\,dx \qquad I_0=\int_0^1 e^{-bx^2}\,dx=\frac{1}{2}\sqrt{\frac{\pi}{b}}\,\mathrm{erf}(\sqrt{b}).$$

$$
\begin{aligned}
I_1 &= \int_0^1 x e^{-bx^2}\,dx \\
&= -\frac{1}{2b}e^{-bx^2}\Big|_0^1 \\
&= \frac{-1}{2b}\left[e^{-b}-1\right]
\end{aligned}
$$

$$
\begin{aligned}
I_2 &= \int_0^1 x^2 e^{-bx^2}\,dx \\
&= -\frac{1}{2b}xe^{-bx^2}\Big|_0^1+\frac{1}{2b}I_0 \\
&= -\frac{1}{2b}e^{-b}+\frac{1}{2b}I_0
\end{aligned}
$$

$$
\begin{aligned}
I_3 &= \int_0^1 x^3 e^{-bx^2}\,dx \\
&= -\frac{1}{2b}x^2e^{-bx^2}\Big|_0^1+\frac{1}{2b}\cdot 2I_1 \\
&= -\frac{1}{2b}e^{-b}+\frac{1}{2b}\cdot 2I_1
\end{aligned}
$$

挖小球：

$$\int_0^{R_n} -\frac{Z}{r}\rho(0)r^2dr\int_0^{2\pi}d\theta\int_0^{\pi}\sin\varphi d\varphi$$

$=-\frac{Z}{2}\rho(0)R_n^2\cdot 2\pi\cdot 2$

$=-2\pi Z\rho(0)R_n^2$

填小球：(均匀带电球体).

$$\int_0^{R_n} -\frac{Z}{R_n}\rho(0)r^2dr\int_0^{2\pi}d\theta\int_0^{\pi}\sin\varphi d\varphi$$

$=-\frac{Z}{R_n}\rho(0)\frac{1}{3}R_n^3\cdot 2\pi\cdot 2$

$=-\frac{4}{3}\pi Z\rho(0)R_n^2$

∴有限核势修正：$-(-2\pi Z\rho(0)R_n^2)+(-\frac{4}{3}\pi Z\rho(0)R_n^2)=\frac{2}{3}\pi Z\rho(0)R_n^2$