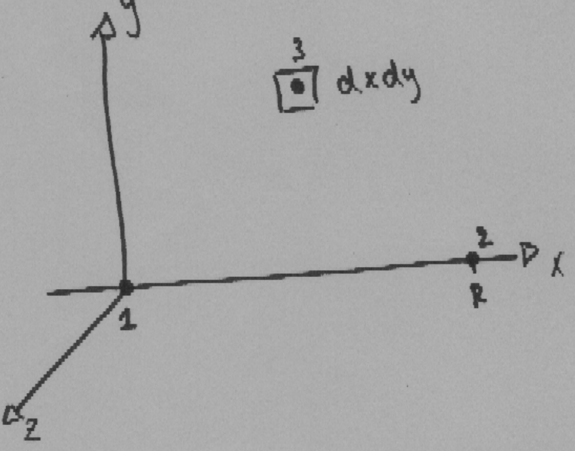
* In order to solve the Kirkwood Equation numerically, it is convenient to use the symmetries in the system and change coordinates such that the 3-dimensional integral over $\vec{r}_3$ becomes a 2-dimensional integral.

Due to the translational symmetry you can choose the position of the origin and due to the ~~spherical~~ rotational symmetry you can choose the orientation of the coordinate system.

=> Place the origin at $\vec{r}_1$, and align the x-axis along $\vec{r}_1 - \vec{r}_2$, such that

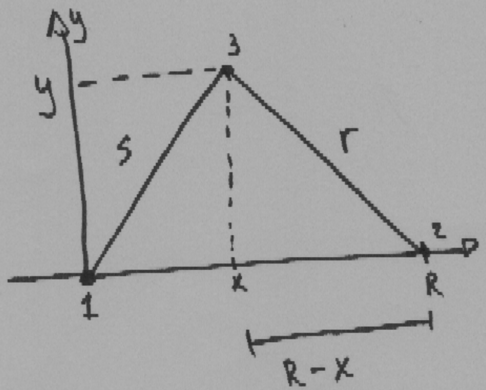
$$\vec{r}_1 = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \qquad \vec{r}_2 = \begin{bmatrix} 0 \\ 0 \\ R \end{bmatrix} \qquad \text{where } R \equiv |\vec{r}_1 - \vec{r}_2|$$



* The integral only depends on $|\vec{r}_1 - \vec{r}_3|$ and $|\vec{r}_2 - \vec{r}_3|$, So it is invariant under rotations about the x-axis. ~~Rotations about~~ Rotating ~~dx~~ the area $dx\,dy$ about the x-axis creates a volume $2\pi y\,dx\,dy$, so the ~~oo~~ volume element $d\vec{r}_3$ becomes $2\pi y\,dx\,dy$, and you only need to integrate over $-\infty \le x \le \infty$ $\quad 0 \le y \le \infty$.

* Make a coördinate transformation from x, y, z to

$R = |\vec{r}_1 - \vec{r}_2|$ ~~&~~ $r = |\vec{r}_2 - \vec{r}_3|$ $s = |\vec{r}_1 - \vec{r}_3|$



So $s = \sqrt{x^2 + y^2}$ $r = \sqrt{y^2 + (R-x)^2}$

* Next, calculate the Jacobian of the transformation

$$J = \det \begin{Bmatrix} \frac{\partial s}{\partial x} & \frac{\partial s}{\partial y} \\ \frac{\partial r}{\partial x} & \frac{\partial r}{\partial y} \end{Bmatrix}$$

$$\frac{\partial s}{\partial x} = \frac{1}{2s} 2x = \frac{x}{s} \qquad \frac{\partial s}{\partial y} = \frac{y}{s}$$

$$\frac{\partial r}{\partial x} = \frac{-2(R-x)}{2r} = \frac{-(R-x)}{r}$$

$$\frac{\partial r}{\partial y} = \frac{y}{r}$$

$$J = \frac{x}{s}\frac{y}{r} + \frac{(R-x)}{r}\frac{y}{s} = \frac{yR}{rs}$$

So $$ds\,dr = \frac{yR}{rs}\,dx\,dy$$

$$dx\,dy = \frac{rs}{yR}\,ds\,dr$$

$$d\vec{r}_3 = 2\pi y\,dx\,dy = 2\pi \frac{rs}{R}\,ds\,dr$$

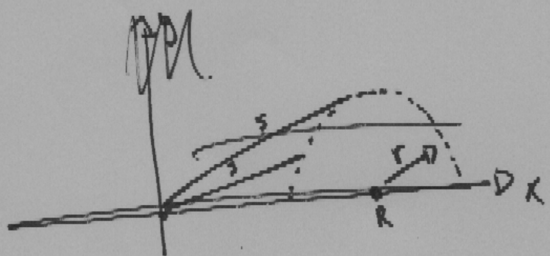
* The domain of integration should cover the upper half of the x-y plane. There are more than one possibilities for the limits of r and s.

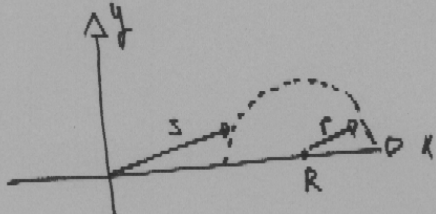
* One possibility is

$$0 \le r \le \infty$$

$$|R-r| \le s \le R+r$$

For a fixed r, the integration over s will be over a semicircle.





r fixes the radius of the dashed semicircle. The integral over s for a fixed r is over the dashed semicircle.

Putting this all together gives

$$-kT\ln g(R;\xi) = \xi u(R) + \frac{2\pi\rho}{R}\int_0^\infty dr\, r[g(r)-1]\int_0^\xi d\xi' \int_{|R-r|}^{R+r} ds\, s\, u(s)\, g(s;\xi')$$

$$-kT\ln\left(g(R;\xi)\right) = \xi u(R) + \frac{2\pi\rho}{R}\int_0^\infty dr\, r[g(r)-1]\int_0^\xi d\xi'\int_{|r-R|}^{r+R} ds\, s\, u(s)\, g(s;\xi')$$

$$R\ln\left(g(R;\xi)e^{\frac{\xi}{kT}u(R)}\right) = -\frac{2\pi}{kT}\rho\int_0^\infty dr\, r[g(r)-1]\int_0^\xi d\xi'\int_{|r-R|}^{r+R} ds\; s\, u(s)\, g(s;\xi')$$

define $Z(R,\xi) \equiv R\ln\left(g(R;\xi)e^{\frac{\xi}{kT}u(R)}\right)$

from the ds integral of the RHS you get $Z(0,\xi)=0$

$$Z'(R;\xi) = -\frac{2\pi}{kT}\rho\int_0^\infty dr\, r[g(r)-1]\int_0^\xi d\xi'\Big[(R+r)u(R+r)g(R+r;\xi')$$
$$-|R-r|u(|r-R|)g(|R-r|;\xi')\,\partial_R|R-r|\Big]$$

$$= -\frac{2\pi}{kT}\rho\int_0^\infty dr\, r[g(r)-1]\int_0^\xi d\xi'\Big[(R+r)u(R+r)g(R+r;\xi')$$
$$+(R-r)u(|R-r|)g(|R-r|;\xi')\Big]$$

$$\Rightarrow \quad Z(R;\xi) = \int_0^R dR'\, Z'(R';\xi)$$

$$g(R;\xi) = \exp\left\{\frac{1}{R}Z(R;\xi) - \frac{\xi}{kT}u(R)\right\}$$