Numerical Solution to the PY equation in Real Space

$$y(|\vec{r}_1-\vec{r}_2|) = 1 + \rho \int d\vec{r}_3 \; f(|\vec{r}_1-\vec{r}_3|)\, y(|\vec{r}_1-\vec{r}_3|)\, h(|\vec{r}_2-\vec{r}_3|)$$

$$y(r) = e^{\beta u(r)} \left[h(r) + 1 \right]$$

$$h(r) = e^{-\beta u(r)} y(r) - 1$$

$$= f(r)\, y(r) + y(r) - 1$$

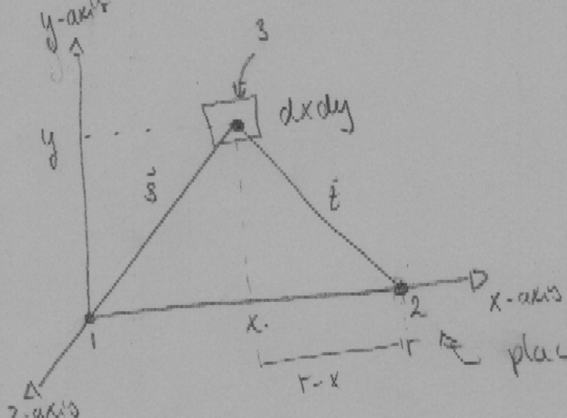
$$y(|\vec{r}_1-\vec{r}_2|) = 1 + \rho \int d\vec{r}_3 \, f(|\vec{r}_1-\vec{r}_3|)\, y(|\vec{r}_1-\vec{r}_3|) \Big\{ f(|\vec{r}_2-\vec{r}_3|)\, y(|\vec{r}_2-\vec{r}_3|) + y(|\vec{r}_2-\vec{r}_3|) - 1 \Big\}$$

place particle 1 at the origin

$$y(|\vec{r}|) = 1 + \rho \int d\vec{s} \; f(|\vec{s}|)\, y(|\vec{s}|) \Big\{ f(|\vec{r}-\vec{s}|)\, y(|\vec{r}-\vec{s}|) + y(|\vec{r}-\vec{s}|) - 1 \Big\}$$

$$|\vec{r}| = |\vec{r}_1 - \vec{r}_2|$$

Coordinates!



place particle 2 on x-axis.

The volume that is created by rotating dxdy around the x-axis is $2\pi y \, dxdy$. So $\int_V d\vec{s} = \int_\Omega 2\pi y \, dxdy$.

where Ω is $-\infty \le x \le \infty$, $0 \le y \le \infty$

change coordinates.

$$r \equiv |\vec{r}_1 - \vec{r}_2|$$

$$s \equiv |\vec{r}_1 - \vec{r}_3|$$

$$t \equiv |\vec{r}_2 - \vec{r}_3|$$

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

Jacobian:

$$J = \det \begin{Bmatrix} \partial s/\partial x & \partial s/\partial y \\ \partial t/\partial x & \partial t/\partial y \end{Bmatrix}$$

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

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

$$\frac{\partial t}{\partial y} = y/t$$

$$J = \frac{x}{s}\frac{y}{t} + \frac{(r-x)}{t}\frac{y}{s} = \frac{ry}{ts}$$

$$dx\,dy = \frac{ts}{ry}\, ds\, dt$$

$$d\vec{S} = 2\pi y\, dx\, dy = 2\pi \frac{ts}{r}\, ds\, dr$$

Boundaries:

$$0 \leq s \leq \infty$$

$$|s-r| \leq t \leq s+r$$

So for fixed s integrate t over the dashed semicircle, and integrate s from 0 to ∞. That will cover the upperhalf of the xy plane.

$$y(r) = 1 + \frac{2\bar{\pi}\rho}{r}\int_0^\infty ds \int_{|s-r|}^{s+r} dt \; st \; f(s)y(s)\left[f(t)y(t) + y(t) - 1\right]$$

$$F(s,t) = f(s)\,y(s)\left[f(t)y(t) + y(t) - 1\right]$$

$$= 1 + \frac{2\bar{\pi}\rho}{r}\int_0^\infty ds \int_{|s-r|}^{s+r} dt \; st \; F(s,t)$$

$$z(r) = r\,y(r)$$

$$z(r) = r + 2\bar{\pi}\rho\int_0^\infty ds \int_{|s-r|}^{s+r} dt \; st \; F(s,t)$$

from this relation it follows that $z(0) = 0$

This equation can be solved numerically, but the s dependence of the boundaries are not nice to implement. This can be avoided by taking a derivative w.r.t. r:

$$z'(r) = \partial_r z(r) = 1 + 2\bar{\pi}\rho\int_0^\infty ds \; s\left[(s+r)F(s,s+r) - |s-r|F(s,|s-r|)\,\partial_r|s-r|\right]$$

$$|s-r|\,\partial_r|s-r| = \frac{1}{2}\,\partial_r(s-r)^2 = -(s-r)$$

$$z'(r) = 1 + 2\bar{\pi}\rho\int_0^\infty ds \; s\left[(s+r)F(s,s+r) + (s-r)F(s,|s-r|)\right]$$

$$F(s,t) = f(s)\,y(s)\,[f(t)\,y(t) + y(t) - 1]$$

$$F(s,t) = \frac{1}{st} f(s)\,z(s)\,[f(t)\,z(t) + z(t) - t]$$

$$z'(r) = 1 + 2\bar{\pi}\rho \int_0^\infty ds \Big\{ f(s)z(s)\,[f(s+r)\,z(s+r) + z(s+r) - (s+r)] + \frac{s-r}{|s-r|} f(s)z(s)\big[f(|s-r|)\,z(|s-r|) + z(|s-r|) - |s-r|\big]\Big\}$$

$$f(s) = e(s) - 1$$

$$z'(r) = 1 + 2\bar{\pi}\rho \int_0^\infty ds\,(e(s)-1)\,z(s)\Big\{ e(s+r)\,z(s+r) + \frac{s-r}{|s-r|}\big[e(|s-r|)\,z(|s-r|)\big] - 2s\Big\} \quad (1)$$

and
$$z(r) = z(0) + \int_0^r dt\ z'(t) \quad (2)$$
$$= \int_0^r dt\ z'(t)$$

$$z(r) = r + 2\bar{\pi}\rho \int_0^r dt \int_0^\infty ds\ (e(s)-1)\,z(s)\Big\{e(s+r)\,z(s+r) + \frac{s-r}{s-r}\big[e(|s-r|)\,z(|s-r|)\big] - 2s\Big\} \quad (3)$$

$$= r + 2\pi\rho\, I[z(r), r]$$

The algorithm is similar to the one in Fourier space.

1) Guess $z_0(r)$ $\left[\text{e.g. } z_0(r) = \lim_{\rho \to 0} z(r) \right]$

2) get $m(r) = r + 2\pi\rho\, I[z_n(r), r]$

3) mix $m(r)$ with $z_n(r)$:

$$z_{n+1}(r) = \alpha\, z_n(r) + (1-\alpha)\, m(r) \qquad 0 \leq \alpha < 1$$

4) Check for convergence
if converged: goto 5
else: goto 2

5) $g(r) = r^{-1} e^{-\beta u(r)}\, z(r)$