I have had no success using the standard iterative method with the potentials for the bosons. The standard iterative method starts with a guess for the densities, then computes the potentials from that guess, then computes new densities from the potentials, and repeats. This works very well when there is only gravity, but I am not really sure why it works at all. It does not seem work well when there is electromagnetism, as far as I can tell this is because small changes in the density can have a a relatively large effect on the electric potential, for example if the electric potential at a point goes from 0.01 to 1. This appears to produce a destabilizing affect in the iteration.

What I propose to do instead is to try to find a SCF using a gradient descent method. Given ρ_e and ρ_a, the electron and alpha densities, the iterative approach would produce $\hat{\rho}_e$ and $\hat{\rho}_p$. I want to minimize

$$\int |\rho_e - \hat{\rho}_e|^2 + |\rho_a - \hat{\rho}_a|^2 \tag{1}$$

or using a discretized grid,

$$f(\rho_{e,j}, \rho_{a,j}, \lambda_a) = \sum_j |\rho_{e,j} - \hat{\rho}_{e,j}|^2 + |\rho_{a,j} - \hat{\rho}_{a,j}|^2 \tag{2}$$

Gradient descent would require at any particular guess for $\rho_{e,i}$, $\rho_{a,i}$, and λ_a computing

$$\frac{\partial f}{\partial \rho_{e,i}} = \sum_j \left[2(\rho_{e,j} - \hat{\rho}_{e,j})(\delta_{ij} - \frac{\partial \hat{\rho}_{e,j}}{\partial \rho_{e,i}}) + 2(\rho_{a,j} - \hat{\rho}_{a,j})(-\frac{\partial \hat{\rho}_{a,j}}{\partial \rho_{e,i}}) \right] \tag{3}$$

$$\frac{\partial f}{\partial \rho_{a,i}} = \sum_j \left[2(\rho_{e,j} - \hat{\rho}_{e,j})(-\frac{\partial \hat{\rho}_{e,j}}{\partial \rho_{a,i}}) + 2(\rho_{a,j} - \hat{\rho}_{a,j})(\delta_{ij} - \frac{\partial \hat{\rho}_{a,j}}{\partial \rho_{a,i}}) \right] \tag{4}$$

$$\frac{\partial f}{\partial \lambda_a} = \sum_j \left[2(\rho_{e,j} - \hat{\rho}_{e,j})(-\frac{\partial \hat{\rho}_{e,j}}{\partial \lambda_a}) + 2(\rho_{a,j} - \hat{\rho}_{a,j})(-\frac{\partial \hat{\rho}_{a,j}}{\partial \lambda_a}) \right] \tag{5}$$

λ_e is not an independent variable as it is always chosen to set $\rho_{e,0} = 1$. Since everything is on a grid, the partials can be easily (although tediously) computed. For now, I am using Boole's rule to compute the potentials:

$$\int_a^b f = \frac{2h}{45} \left[7f(a) + 32f(a+h) + 12f(a+2h) + 32f(a+3h) + 14f(a+4h) + 32f(a+5h) + ... \right] \tag{6}$$

The potentials are usually expanded into Legendre polynomials, but since there is radial symmetry, we are just left with

$$\int \frac{(m_e \rho_e^{3/2} + m_a \rho_a^2)(y)}{|x-y|} d^3y = 2\pi \int_0^\infty f_0(r', r)(m_e \rho_e^{3/2}(r') + m_a \rho_a^2(r')) dr' \tag{7}$$

where we have assumed equatorial symmetry and

$$f_{2n}(r', r) = \begin{cases} r'^{2n+2}/r^{2n+1} & r' < r \\ r^{2n}/r'^{2n-1} & r < r' \end{cases}$$

Boole's rule then approximates this with

$$G(r) = 2\pi \frac{2h}{45} \left[7f_0(0, r)(m_e \rho_e^{3/2}(0) + m_a \rho_a^2(0)) + 32f_0(h, r)(m_e \rho_e^{3/2}(h) + m_a \rho_a^2(h)) + ... \right] \tag{8}$$

Likewise,

$$E(r) = 2\pi \frac{2h}{45} \left[7f_0(0, r)(2\rho_a^2(0) - \rho_e^{3/2}(0)) + 32f_0(h, r)(2\rho_a^2(h) - \rho_e^{3/2}(h)) + ... \right] \tag{9}$$

So that on a discretized grid, we have

$$G_j = 2\pi\frac{2h}{45}\left[7f_0(r_0,r_j)(m_e\rho_{e,0}^{3/2}+m_a\rho_{a,0}^2)+32f_0(r_1,r_j)(m_e\rho_{e,1}^{3/2}+m_a\rho_{a,1}^2)+...\right] \tag{10}$$

and

$$E_j = 2\pi\frac{2h}{45}\left[7f_0(r_0,r_j)(2\rho_{a,0}^2-\rho_{e,0}^{3/2})+32f_0(r_1,r_j)(2\rho_{a,1}^2-\rho_{e,1}^{3/2})+...\right] \tag{11}$$

$\hat{\rho}_{e,j}$ is defined as

$$\hat{\rho}_{e,j} = \max\left((-\hat{\lambda}_e+m_eG_j+e^2E_j)\frac{2m_e3^{2/3}\pi^{4/3}}{\hbar^2},0\right) \tag{12}$$

where

$$\hat{\lambda}_e = m_eG_0+e^2E_0-\frac{\hbar^2}{2m_e3^{2/3}\pi^{4/3}} \tag{13}$$

is chosen so that $\hat{\rho}_{e,0}=1$. Then we can compute

$$\frac{\partial\hat{\rho}_{e,j}}{\partial\rho_{e,i}} = \begin{cases}\left(-m_e\frac{\partial G_0}{\partial\rho_{e,i}}-e^2\frac{\partial E_0}{\partial\rho_{e,i}}+m_e\frac{\partial G_j}{\partial\rho_{e,i}}+e^2\frac{\partial E_j}{\partial\rho_{e,i}}\right)\frac{2m_e3^{2/3}\pi^{4/3}}{\hbar^2} & \text{else}\\ 0 & \hat{\rho}_{e,j}=0\end{cases}$$

$$\frac{\partial\hat{\rho}_{e,j}}{\partial\rho_{a,i}} = \begin{cases}\left(-m_e\frac{\partial G_0}{\partial\rho_{a,i}}-e^2\frac{\partial E_0}{\partial\rho_{a,i}}+m_e\frac{\partial G_j}{\partial\rho_{a,i}}+e^2\frac{\partial E_j}{\partial\rho_{a,i}}\right)\frac{2m_e3^{2/3}\pi^{4/3}}{\hbar^2} & \text{else}\\ 0 & \hat{\rho}_{e,j}=0\end{cases}$$

$$\frac{\partial\hat{\rho}_{e,j}}{\partial\lambda_a} = 0 \tag{14}$$

$$\frac{\partial E_j}{\partial\rho_{e,i}} = -2\pi\frac{2h}{45}K_if_0(r_i,r_j)\frac{3}{2}\rho_{e,i}^{1/2} \tag{15}$$

$$\frac{\partial G_j}{\partial\rho_{e,i}} = 2\pi\frac{2h}{45}K_if_0(r_i,r_j)\frac{3}{2}m_e\rho_{e,i}^{1/2} \tag{16}$$

$$\frac{\partial E_j}{\partial\rho_{a,i}} = 2\pi\frac{2h}{45}K_if_0(r_i,r_j)4\rho_{a,i} \tag{17}$$

$$\frac{\partial G_j}{\partial\rho_{a,i}} = 2\pi\frac{2h}{45}K_if_0(r_i,r_j)2m_a\rho_{a,i} \tag{18}$$

where K_i is the coefficient from the integration scheme.

The alpha particles are more difficult, here we use just Euler's method for simplicity, but the idea is clearly the same for other methods. With Euler's, we have

$$\hat{\rho}_{a,j} = \hat{\rho}_{a,j-1}+h\hat{\rho}'_{a,j-1} \tag{19}$$

and

$$\hat{\rho}'_{a,j} = \hat{\rho}'_{a,j-1}+h\left[-\frac{2}{r_{j-1}}\hat{\rho}'_{a,j-1}+\hat{\rho}_{a,j-1}\frac{2m_a}{\hbar^2}\left(\lambda_a-m_aG_{j-1}+2e^2E_{j-1}\right)\right] \tag{20}$$

$$\frac{\partial\hat{\rho}_{a,j}}{\partial\rho_{e,i}} = \frac{\partial\hat{\rho}_{a,i-1}}{\partial\rho_{e,i}}+h\frac{\partial\hat{\rho}'_{a,i-1}}{\partial\rho_{e,i}} \tag{21}$$

$$\frac{\partial\hat{\rho}_{a,j}}{\partial\rho_{a,i}} = \frac{\partial\hat{\rho}_{a,i-1}}{\partial\rho_{a,i}}+h\frac{\partial\hat{\rho}'_{a,i-1}}{\partial\rho_{a,i}} \tag{22}$$

$$\frac{\partial \hat{\rho}'_{a,j}}{\partial \rho_{e,i}} = \frac{\partial \hat{\rho}'_{a,j-1}}{\partial \rho_{e,i}} \left[1 - h\frac{2}{r_{j-1}}\right] + h\frac{\partial \hat{\rho}_{a,j-1}}{\partial \rho_{e,i}} \frac{2m_a}{\hbar^2} \left[\lambda_a - m_a G_{j-1} + 2e^2 E_{j-1}\right] \tag{23}$$

$$+ h\hat{\rho}_{a,j-1} \frac{2m_a}{\hbar^2} \left[-m_a \frac{\partial G_{j-1}}{\partial \rho_{e,i}} + 2e^2 \frac{\partial E_{j-1}}{\partial \rho_{e,i}}\right] \tag{24}$$

$$\frac{\partial \hat{\rho}'_{a,j}}{\partial \rho_{a,i}} = \frac{\partial \hat{\rho}'_{a,j-1}}{\partial \rho_{a,i}} \left[1 - h\frac{2}{r_{j-1}}\right] + h\frac{\partial \hat{\rho}_{a,j-1}}{\partial \rho_{a,i}} \frac{2m_a}{\hbar^2} \left[\lambda_a - m_a G_{j-1} + 2e^2 E_{j-1}\right] \tag{25}$$

$$+ h\hat{\rho}_{a,j-1} \frac{2m_a}{\hbar^2} \left[-m_a \frac{\partial G_{j-1}}{\partial \rho_{a,i}} + 2e^2 \frac{\partial E_{j-1}}{\partial \rho_{a,i}}\right] \tag{26}$$

$$\frac{\partial \hat{\rho}'_{a,j}}{\partial \lambda_a} = \frac{\partial \hat{\rho}'_{a,j-1}}{\partial \lambda_a} \left[1 - h\frac{2}{r_{j-1}}\right] + h\frac{\partial \hat{\rho}_{a,j-1}}{\partial \lambda_a} \frac{2m_a}{\hbar^2} \left[\lambda_a - m_a G_{j-1} + 2e^2 E_{j-1}\right] + h\hat{\rho}_{a,j-1} \frac{2m_a}{\hbar^2} \tag{27}$$

With these calculations, we can then take some small step in the direction $-\nabla f$, decreasing f and hopefully after many steps arriving to some point at which f evaluates to a small number.