

Appendix E Generalized Variational Theory of Reaction Rates

Inspired by the geometrical interpretation of the BBGKY hierarchy, we start by asking what is the flow out of a region $R \subset T^*M^n$ if we are given the $\tilde{\rho}^{(n+1)}$, the $n+1$ particle distribution form. This flow is

$$\begin{aligned} \frac{dN^{(n)}}{dt} &= \frac{1}{V^n} \int_R \frac{\partial \rho^{(n)}}{\partial t} + \mathcal{L}_{u^{(n)}} \rho^{(n)} \\ &= -\frac{n_0}{V^n} \int_{R \times T^*M} \mathcal{L}_{u_{int}^{(n)}} \tilde{\rho}^{(n+1)} \\ &= -\frac{n_0}{V^n} \int_{\partial(R \times T^*M)} i_{u_{int}^{(n)}} \tilde{\rho}^{(n+1)} \end{aligned}$$

where the region R is convected by the n -particle flow. Making the assumption

$$i_{u_{int}^{(n)}} \tilde{\rho}^{(n+1)} \Big|_{R \times \partial(T^*M)} = 0$$

we find that the flux is

$$\frac{dN^{(n)}}{dt} = -\frac{n_0}{V^n} \int_{\partial R \times T^*M} i_{u_{int}^{(n)}} \tilde{\rho}^{(n+1)}$$

Assume that we can construct a continuous function g on T^*M^n advected by the flow $\mathcal{L}_{u^{(n)}} g = 0$. At least one such function exists since $\mathcal{L}_{u^{(n)}} H^{(n)} = 0$. One can foliate T^*M^n by use of g and leaves of this foliation are invariant under the flow $u^{(n)}$.

Now consider a region R whose boundary is given by two sets of leaves S_0 and S_1 .

Define interior set of leaves S which divide R into two regions R_0 and R_1 such that $S+S_0=\partial R_0$ and $S+S_1=\partial R_1$. Define the bottleneck set, S_b , as the interior set that gives the minimum value of the absolute flux, Φ_b .

$$\frac{n_0}{V^n} \int_{S \times T^*M} |i_{u_{int}^{(n)}} \tilde{\rho}^{(n+1)}| \geq \Phi_b = \frac{n_0}{V^n} \int_{S_b \times T^*M} |i_{u_{int}^{(n)}} \tilde{\rho}^{(n+1)}| \quad \forall S$$

If $\tilde{\rho}^{(n+1)}$ is upper bound $\rho^{(n+1)}$, that is

$$\int_A \rho^{(n+1)} \leq \int_A \tilde{\rho}^{(n+1)} \quad \forall \rho^{(n+1)} \text{ and } A \subset T^*M^{n+1}$$

then steady state flux must be less than Φ_b

Proof starts by assuming that there is a steady state flux greater than Φ_b . Separating R into two regions by S_b , one can readily see that $\rho^{(n+1)}$ will increase one of these regions until it must exceed the upper bound $\tilde{\rho}^{(n+1)}$.

Φ_b is variational estimate of the rate, the variation being over all interior sets of leaves, S , and the rate being the steady state flux through R .

There are two practical limitations: (1) the range of S varied over, (2) order of $\tilde{\rho}^{(n+1)}$.

Most common apps $\tilde{\rho}^{(2)}$ and S_E such that $H^{(1)} = E$. For this case

$$\Phi_b = \frac{n_0}{V} \int_{S_E \times T^*M} |i_{u_{12}} \tilde{\rho}^{(2)}|$$

Pulling this back (see Appendix C) one gets

$$\Phi_b = \frac{n_0}{V} \int_{E=H_1(p, q_1)} dq_1 dp_2 dq_2 \tilde{f}_2 \left| \left[H_{12}, H \right] \frac{\partial P_1}{\partial H_1} \right|$$

Recombination in constant $\vec{B} = B\hat{z}$ of massive ion $m_i \rightarrow \infty$ with constant $v_{i\perp}$

Constant $v_{i\perp}$ equivalent to stationary ion with constant electric field $\vec{E} = m_e \Omega_e (\vec{v}_i \times \hat{z}) = \frac{e}{c} \vec{v}_i \times \vec{B}$
 $E_0 = m_e \Omega_e \bar{v}_{i\perp} = eB\bar{v}_{i\perp}/c$

See App. B for derivation of Hamiltonian

$$H_1(z, p_z, x, p_x) = \frac{p_z^2}{2m} - \frac{e^2}{\sqrt{x^2 + \left(\frac{p_x}{m\Omega}\right)^2 + z^2}} + eE_0 x$$

where $\vec{B} = (mc\Omega/e)\hat{z}$ $\vec{E} = E_0\hat{x}$ and $z = p_x/m\Omega$

The interaction Hamiltonian is given by

$$H_{12} = \frac{e^2}{\sqrt{(x_1 - x_2)^2 + \left(\frac{p_{x1} - p_{x2}}{m\Omega}\right)^2 + (z_1 - z_2)^2}} \equiv r_{12}$$

First we turn our attention to the case of the stationary ion $\bar{v}_{i\perp} \rightarrow 0$. The easiest way to guarantee this is to have $T_i \ll T_e$.

We anticipate the existence of a bottleneck for this case and set $\tilde{f}_2$ equal to zero for $H_1 < E$ and equal to thermal distribution for $H_1 > E$

$$\tilde{f}_2 \sim \frac{N}{2\pi(m\bar{v})^2(m\Omega)^2} e^{-(H_1 + H_2 + H_{12})}$$

Now we calculate

$$\frac{d\rho_{12}}{dH_1} = \frac{m}{\rho_{12}}$$

$$\{H_{12}, H_1\} = \frac{e^2}{m} \frac{\rho_{12}(z_1 - z_2)}{r_{12}^3} + \left(\frac{e^2}{m\Omega}\right)^2 \left(\frac{x_2 p_{1x} - x_1 p_{2x}}{r_{12}^3 r_{12}^3}\right)$$

$$= (\vec{p}_1 \cdot \vec{F}_{12})_{1 \rightarrow B} + (\vec{p}_1 \cdot \vec{F}_{12})_{1 \rightarrow B} \text{ (i.e. } \vec{E} \times \vec{B} \text{ dot)} \\ = \frac{dK_{11}}{dt} + \frac{dK_1}{dt}$$

Note constraints:

- (1) $H_1 = -E_s$ (at bottleneck or separatrix)
- (2) $H \geq -E_s$ (particle $\neq z$ unbound)
- (3) $i v_{vol}^2 \approx 0$ ($\tilde{f}_2 = 0$ below)
- (4) $\bar{\rho}_{12} \leq \rho_0$ (adiabatic bottleneck cutoff to limit multiple crossings)

$$\Phi_b = \frac{n}{V} \int \frac{N}{2\pi(mv)^2(m\Omega)^2} e^{-(H_1+H_2+H_{12})} \begin{matrix} (2) & (2) \\ \pm p_{1x} & \pm p_{2x} \end{matrix} \left[\frac{e^2(z_1-z_2)}{r_{12}^3} + \frac{m}{\rho_{12}} \left(\frac{e^2}{m\Omega} \right)^2 \left(\frac{x_2 p_{1x} - x_1 p_{2x}}{r_1^3 r_2^3} \right) \right] dx_1 dz_1 dp_{1x} d\rho_{1z} dx_2 dz_2 dp_{2x} d\rho_{2z}$$

Now make the change of variables (dimensionless) to:

$$\begin{cases} \varepsilon_s \equiv -\frac{E_s}{m\bar{v}^2} & \rho_1 \equiv r_1/b & \bar{x} \equiv x/b \\ \varepsilon_2 \equiv \frac{p_{2z}^2}{2m\bar{v}^2} & \rho_2 \equiv r_2/b & \bar{y} \equiv p_{1x}/m\Omega b \\ \mu_2 \equiv \frac{1}{\rho_2} - \frac{1}{\rho_{12}} & \rho_{12} \equiv r_{12}/b & \bar{z} \equiv z/b \\ b = \frac{e^2}{m\bar{v}^2} & \vec{r}_{12} = \vec{x}_1 - \vec{x}_2 & \\ r_{ce}^2 = \left(\frac{\bar{v}}{\Omega} \right)^2 & & \end{cases}$$

$$= n^2 \bar{v} b^5 \frac{4}{2\pi\sqrt{2}} e^{\varepsilon_s} \int_{s^7} e^{-\varepsilon_2 + \mu_2} \left[\frac{\bar{z}_1 - \bar{z}_2}{\rho_{12}^3} + \left(\frac{r_{ce}}{\sqrt{2}b} \right) \frac{\bar{x}_2 \bar{y}_1 - \bar{x}_1 \bar{y}_2}{\rho_1^3 \rho_{12}^3 \sqrt{\frac{1}{\rho_1} - \varepsilon_s}} \right] \varepsilon_2^{-1/2} d\varepsilon_2 d\bar{x} d\bar{y} d\bar{z} d\bar{x}_2 d\bar{y}_2 d\bar{z}_2$$

Let us concentrate on doing the ε_2 integral

$$\begin{aligned} & \xrightarrow{\pm p_{2z}} \pm \varepsilon_2^{1/2} \rightarrow 2 \int_{\max(0, \mu_2)}^{\infty} e^{-\varepsilon_2} \varepsilon_2^{-1/2} d\varepsilon_2 \\ & = 2\sqrt{\pi} \operatorname{erfc}(\sqrt{\max(0, \mu_2)}) \\ & \equiv F(\mu_2) \end{aligned}$$

Since particle #2 is not bound $H = H_1 + H_2 + H_{12} \geq -E_s$

$$\Rightarrow -\varepsilon_s + \varepsilon_2 - \mu_2 \geq -\varepsilon_s$$

$$\Rightarrow \varepsilon_2 \geq \mu_2$$

which gives the lower bound on integral

So

$$\Phi_b = \frac{n^2 \bar{v} b^5}{\pi\sqrt{2}} e^{\varepsilon_s} \int_{s^6} F(\mu_2) e^{\mu_2} \left[\frac{(\vec{\rho}_{12})_z}{\rho_{12}^3} + \left(\frac{r_{ce}}{\sqrt{2}b} \right) \frac{(\vec{\rho}_1 \times \vec{\rho}_{12})_z}{\rho_1^3 \rho_{12}^3 \sqrt{\frac{1}{\rho_1} - \varepsilon_s}} \right] d\bar{x} d\bar{y} d\bar{z} d\bar{x}_2 d\bar{y}_2 d\bar{z}_2$$

Now change to spherical coordinates for $\vec{\rho}_1$ and $\vec{\rho}_2$

from $(\vec{\rho}_1, \vec{\rho}_2) = (\bar{x}_1, \bar{y}_1, \bar{z}_1, \bar{x}_2, \bar{y}_2, \bar{z}_2)$ to $(\bar{\rho}_1, \xi, \psi, \bar{\rho}_{12}, \theta, \varphi)$

where

$$\vec{\rho}_1 - \vec{\rho}_2 = \bar{\rho}_{12} \varepsilon_s^{-1} (\sin\theta \cos\psi \hat{x} + \sin\theta \sin\psi \hat{y} + \cos\theta \hat{z})$$

$$\vec{\rho}_1 = \bar{\rho}_1 \varepsilon_s^{-1} (\sin\xi \cos\psi \hat{x}' + \sin\xi \sin\psi \hat{y}' + \cos\xi \hat{z}')$$

and

$$\hat{z}' = \sin\theta \cos\psi \hat{x} + \sin\theta \sin\psi \hat{y} + \cos\theta \hat{z}$$

$$\hat{y}' = -\sin\psi \hat{x} + \cos\psi \hat{y}$$

$$\hat{x}' = \cos\theta \cos\psi \hat{x} + \cos\theta \sin\psi \hat{y} - \sin\theta \hat{z}$$

$$\Phi_b = \frac{n^2 \bar{v} b^5}{\pi \sqrt{2}} \frac{\varepsilon_s^{\xi}}{\varepsilon_s^4} \int_{S^b} F(\mu_2) e^{\mu_2} \left[\frac{\cos\theta}{\bar{\rho}_{12}^2} + \frac{\sin\theta \sin\xi \cos\psi}{\bar{\rho}_1^2 \bar{\rho}_{12}^2 \varepsilon_s^{3/2} \sqrt{\frac{1}{\bar{\rho}_1} - 1}} \left(\frac{r_{ce}}{\sqrt{2} b} \right) \right] \bar{\rho}_{12}^2 d\bar{\rho}_{12} d\psi d(\cos\theta) \bar{\rho}_1^2 d\bar{\rho}_1 d\psi d(\cos\xi)$$

with limits of integration:

$$0 \leq \bar{\rho}_{12} \leq \infty \quad 0 \leq \bar{\rho}_1 \leq \infty$$

$$0 \leq \psi \leq 2\pi \quad 0 \leq \psi \leq 2\pi$$

$$-1 \leq \cos\theta \leq 1 \quad 0 \leq \cos\xi \leq 2\pi$$

with additional 3 constraints

$$i_v \text{ vol} \geq 0 \quad (\#3) \quad \text{one way flux}$$

$$\bar{\rho}_1 \leq 1 \quad (\#1) \quad \text{on energy surface } \varepsilon_s = \text{const}$$

$$\bar{\rho}_{12} \leq \rho_0 \quad (\#4) \quad \text{adiabatic cutoff}$$

Do ψ integration

$$\Phi_b = n^2 \bar{v} b^5 \sqrt{2} \frac{e^{\xi}}{\varepsilon_s^4} \int_{S^b} F(\mu_2) e^{\mu_2} \bar{\rho}_1^2 \left[\cos\theta + \sin\theta \left(\frac{\sin\xi \cos\psi}{\varepsilon_s^{3/2} \bar{\rho}_1 \sqrt{\bar{\rho}_1(1-\bar{\rho}_1)}} \right) \left(\frac{r_{ce}}{\sqrt{2} b} \right) \right] d\bar{\rho}_1 d\bar{\rho}_{12} d(\cos\theta) d\psi d(\cos\xi)$$

Now do θ integration subject to the constraint that $i_v \text{ vol} \geq 0$ or $\cos\theta + C \sin\theta \geq 0$ where

$$C \equiv \varepsilon_s^{3/2} \frac{\sin\xi \cos\psi}{\bar{\rho}_1 \sqrt{\bar{\rho}_1(1-\bar{\rho}_1)}} \left(\frac{r_{ce}}{\sqrt{2} b} \right)$$

Define

$$G(C) \equiv \int_{\cos \theta + C \sin \theta \geq 0} \cos \theta + C \sin \theta \, d(\cos \theta)$$

$$\cos \theta + C \sin \theta \geq 0$$

$$= \int_{\cos \theta = \frac{-C}{\sqrt{1+C^2}}}^1 \cos \theta + C \sin \theta \, d(\cos \theta)$$

$$\cos \theta = \frac{-C}{\sqrt{1+C^2}}$$

$$= \left[\frac{\cos^2 \theta}{2} - C \left(-\frac{1}{2} \cos \theta \sin \theta + \frac{\theta}{2} \right) \right]_{\cos \theta = \frac{-C}{\sqrt{1+C^2}}}^1$$

$$\cos \theta = \frac{-C}{\sqrt{1+C^2}}$$

$$= \frac{1}{2} \left[1 + C \cos^{-1} \left(\frac{-C}{\sqrt{1+C^2}} \right) \right] \quad (0 \leq \cos^{-1} x \leq \pi)$$

$$= \frac{1}{2} \left[1 + C \cot^{-1}(-C) \right] \quad (0 \leq \cot^{-1} x \leq \pi)$$

Use the definition of $G(C)$ and do the θ integral

$$\Phi_b = n \bar{v} b^5 \sqrt{2} \frac{e^{\xi_s}}{\xi_s^4} \int_{S^4} F(\mu_2) e^{\mu_2} G(C) \bar{\rho}_1^2 d\bar{\rho}_1 d\bar{\rho}_2 d\psi d(\cos \xi)$$

Define

$$\bar{G}(a) \equiv \int_0^{2\pi} G(a \cos \psi) d\psi = \pi (1+a)$$

Use this definition to do the ψ integral giving:

$$\Phi_b = n \bar{v} b^5 \sqrt{2} \frac{e^{\xi_s}}{\xi_s^4} \int_{S^3} F(\mu_2) e^{\mu_2} \bar{G}(a) \bar{\rho}_1^2 d\bar{\rho}_1 d\bar{\rho}_2 d(\cos \xi)$$

$$\text{where } a \equiv \varepsilon_s^{3/2} \frac{\sin \xi}{\bar{\rho}_1 \sqrt{\bar{\rho}_1(1-\bar{\rho}_1)}} \left(\frac{r_{ce}}{\sqrt{2} b} \right)$$

Let's now explicitly put in the limits of integration

$$\bar{\Phi}_b = R_0 (2\pi)^{3/2} \frac{e^{\varepsilon_s}}{\varepsilon_s^4} \int_{\bar{\rho}_1=0}^1 \bar{\rho}_1^2 d\bar{\rho}_1 \int_{\cos \xi=-1}^1 d(\cos \xi) \bar{G}(a) \int_{\bar{\rho}_{12}=0}^{\rho_0} d\bar{\rho}_{12} \bar{F}(\mu_2)$$

where

$$R_0 = n^2 \bar{v} b^5$$

$$a \equiv \varepsilon_s^{3/2} \left(\frac{r_{ce}}{\sqrt{2} b} \right) \frac{\sin \xi}{\bar{\rho}_1 \sqrt{\bar{\rho}_1(1-\bar{\rho}_1)}}$$

$$\mu_2 \equiv \varepsilon_s \left(\frac{1}{\bar{\rho}_2} - \frac{1}{\bar{\rho}_{12}} \right) = \varepsilon_s \frac{\bar{\rho}_{12} - \bar{\rho}_2}{\bar{\rho}_2 \bar{\rho}_{12}}$$

$$\bar{\rho}_2^2 = \bar{\rho}_1^2 + \bar{\rho}_{12}^2 - 2 \bar{\rho}_1 \bar{\rho}_{12} \cos \xi$$

$$\bar{F}(\mu_2) \equiv e^{\mu_2} \operatorname{erfc}(\sqrt{\max(0, \mu_2)})$$

$$\bar{G}(a) \equiv (1+a)$$

$$= R_0 \frac{e^{\varepsilon_s}}{\varepsilon_s^4} f\left(\frac{r_{ce}}{\sqrt{2} b}, \varepsilon_s, \rho_0\right)$$

if $r_{ce} \ll b \varepsilon_s^{-3/2}$ then

$$\bar{\Phi}_b = R_0 \frac{e^{\varepsilon_s}}{\varepsilon_s^4} f(0, \varepsilon_s, \rho_0)$$

$$= R_0 \frac{e^{\varepsilon_s}}{\varepsilon_s^4} g(\varepsilon_s, \rho_0)$$

where

$$g(\varepsilon_s, \rho_0) = (2\pi)^{3/2} \int_{\bar{\rho}_1=0}^1 \bar{\rho}_1^2 d\bar{\rho}_1 \int_{\bar{\rho}_{12}=0}^{\rho_0} d\bar{\rho}_{12} \int_{x=-1}^1 dx \bar{F}(\mu_2)$$

and $X = \cos \xi$, $\mu_2 = \epsilon_s \frac{\bar{\rho}_{12} - \bar{\rho}_2}{\bar{\rho}_{12} \bar{\rho}_2}$, $\bar{\rho}_2^2 = \bar{\rho}_1^2 + \bar{\rho}_{12}^2 - 2\bar{\rho}_1 \bar{\rho}_{12} X$

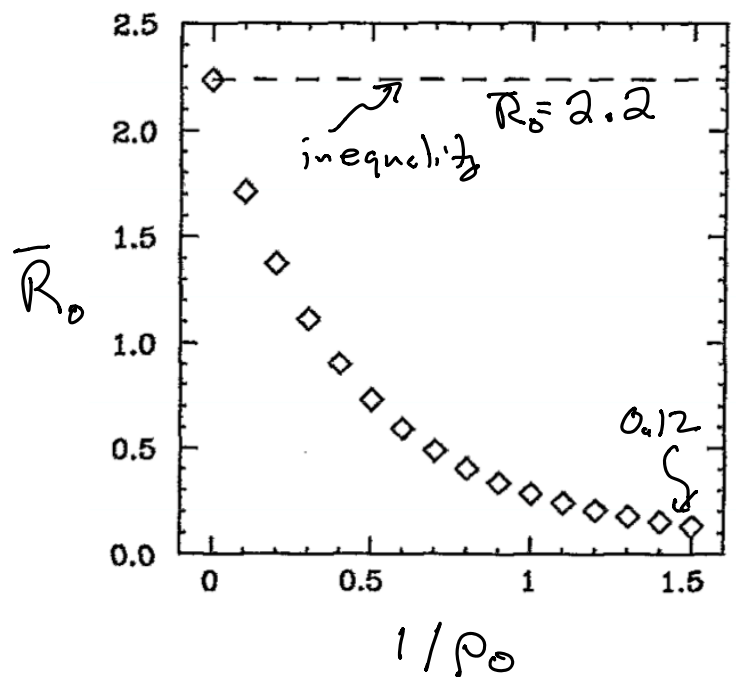
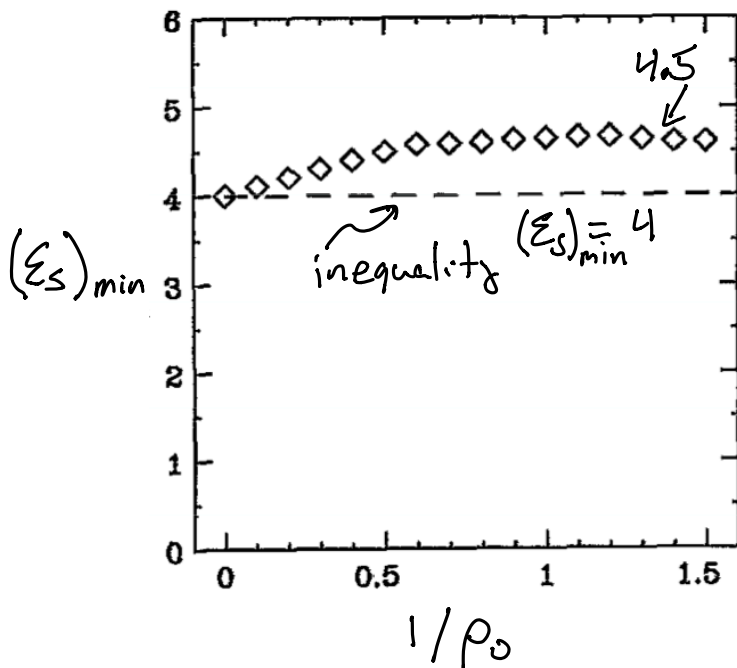
$$\bar{F}(\mu_2) = e^{\mu_2} \text{erfc}(\sqrt{\max(0, \mu_2)})$$

Using the inequality $\bar{F}(\mu_2) \leq 1$ and evaluating the integrals in yields

$$\bar{\Phi}_b \leq R_0 \frac{e^{\epsilon_s}}{\epsilon_s^4} \frac{2(2\pi)^{3/2}}{3} \rho_0 \quad \text{for equality } 1/\rho_0 = 0$$

$$(\bar{\Phi}_b)_{\min} @ (\epsilon_s)_{\min} = R_0 \rho_0 \bar{R}_0 \left(\frac{1}{\rho_0} \right)$$

for the inequality $(\epsilon_s)_{\min} = 4$ and $\bar{R}_0 = \frac{e^4}{4^4} \frac{2(2\pi)^{3/2}}{3} \approx 2.2$



Note the correction to $\bar{\Phi}_b$ due to $\perp E \times B$ drift is of order $\frac{\omega_{E \times B}}{\omega_z} = \left(\frac{r_{ce}}{r_0} \right) \epsilon_s^{3/2}$ when compared to the $\parallel z$ flux.

If there is a separatrix at $\bar{r}_s \sim \xi_s^{-1}$ and the distribution is thermal @ $\bar{r}_{ci}$. Then $e^{\xi_s} \rightarrow e^{1/\bar{r}_{ci}}$ and $\xi_s \rightarrow \bar{r}_s^{-1}$. Note that $(\xi_s)_{\min}$ asymptotes to 4.5. This will be the case if $v_{it} \neq 0$, that is $E_0 \neq 0$. See app. B for details,

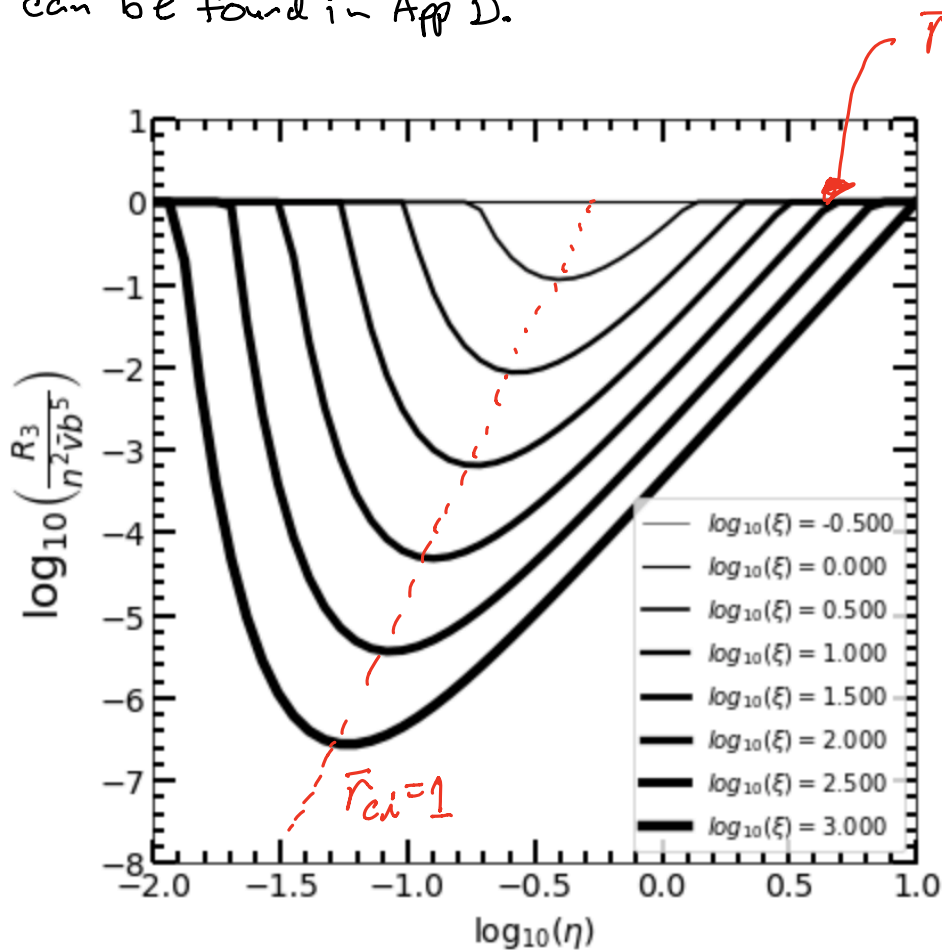
Therefore,

$$(\Phi_b)_{\bar{r}_s} \sim R_0 \max\left(1, e^{1/\bar{r}_{ci}} \left(\mathcal{O}[\bar{r}_s^{-9/2}] + \mathcal{O}\left[\underbrace{\left(\frac{r_{ce}}{b}\right)^{-3/2}}_{\frac{\omega_{D1}}{\omega_{Z1}}} \bar{r}_s^{-9/2}\right] \right)\right)$$

A similar result is shown in App B where the separatrix is at

$$\bar{r}_s = \left(\frac{v_i}{v_e} \frac{b}{r_{ce}} \right)^{-1/2} = \left(\frac{T_i}{T_e} \right)^{-1/4} \left[\left(\frac{m_e}{m_i} \right)^{1/2} \frac{b}{r_{ce}} \right]^{1/2}$$

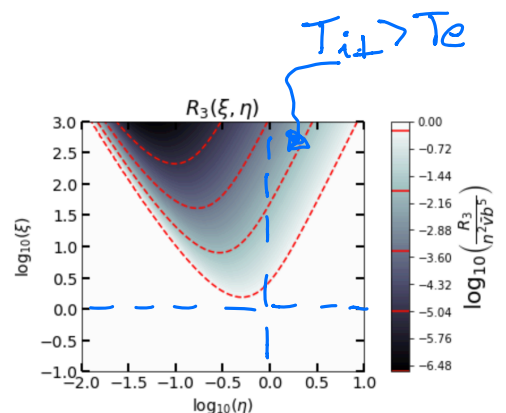
Details of the calculation can be found in App D.



$$\frac{(\Phi_b)_{\bar{r}_s}}{R_0} = \frac{R_3}{n^2 b^5 \bar{v}}$$

$$\xi \equiv \frac{T_{it}}{T_e}$$

$$\eta \equiv \left[\left(\frac{r_{ce}}{b} \right)^2 \frac{m_i}{m_e} \right]^{1/3} = \left(\frac{\omega_p}{\Omega_i} \right)^{1/3}$$



Let us now separate the terms without $\frac{r_{ce}}{r_2 b} \varepsilon_s^{3/2} \equiv \varepsilon$ dependence and the one that is linear in ε .

$$\bar{\Phi}_b = R_0 \frac{e \varepsilon_s}{\varepsilon_s^4} \left[g(\varepsilon_s, \rho_0) + \left(\frac{r_{ce}}{r_2 b} \right) \varepsilon_s^{3/2} h(\varepsilon_s, \rho_0) \right]$$

$$g(\varepsilon_s, \rho_0) = (2\pi)^{3/2} \int_{\bar{\rho}_1=0}^1 \bar{\rho}_1^2 d\bar{\rho}_1 \int_{\bar{\rho}_{12}=0}^{\rho_0} d\bar{\rho}_{12} \int_{x=-1}^1 dx \bar{F}(\mu_2)$$

and

$$h(\varepsilon_s, \rho) = (2\pi)^{3/2} \int_{\bar{\rho}_1=0}^1 \frac{\bar{\rho}_1 d\bar{\rho}_1}{\sqrt{\bar{\rho}_1(1-\bar{\rho}_1)}} \int_{\bar{\rho}_{12}}^{\rho_0} d\bar{\rho}_{12} \int_{x=-1}^1 dx \sqrt{1-x^2} \bar{F}(\mu_2)$$

Now onto the more detailed evaluation of $f\left(\frac{r_{ce}}{r_2 b}, \varepsilon_s, \rho_0\right)$, $g(\varepsilon_s, \rho_0)$ and $h(\varepsilon_s, \rho_0)$

$$f\left(\frac{r_{ce}}{r_2 b}, \varepsilon_s, \rho_0\right) = (2\pi)^{3/2} \int_{\bar{\rho}_1=0}^1 \bar{\rho}_1^2 d\bar{\rho}_1 \int_{\cos \xi=-1}^1 d(\cos \xi) \bar{G}(a) \int_{\bar{\rho}_{12}=0}^{\rho_0} d\bar{\rho}_{12} \bar{F}(\mu_2)$$

$$a \equiv \varepsilon_s^{3/2} \left(\frac{r_{ce}}{r_2 b} \right) \frac{\sin \xi}{\bar{\rho}_1 \sqrt{\bar{\rho}_1(1-\bar{\rho}_1)}}$$

$$\mu_2 \equiv \varepsilon_s \left(\frac{1}{\bar{\rho}_2} - \frac{1}{\bar{\rho}_{12}} \right) = \varepsilon_s \frac{\bar{\rho}_{12} - \bar{\rho}_2}{\bar{\rho}_2 \bar{\rho}_{12}}$$

$$\bar{\rho}_2^2 = \bar{\rho}_1^2 + \bar{\rho}_{12}^2 - 2 \bar{\rho}_1 \bar{\rho}_{12} \cos \xi$$

$$\bar{F}(\mu_2) \equiv e^{\mu_2} \operatorname{erfc}(\sqrt{\max(0, \mu_2)})$$

$$\bar{G}(a) \equiv 1 + a$$

$$\varepsilon = \frac{\varepsilon_S^{3/2}}{r^2} \left(\frac{r_{ce}}{b} \right) \quad \bar{\varepsilon} = 1/\rho_0 \quad \bar{\bar{\varepsilon}} = \varepsilon_S^{1/2}/\rho_0$$

So

$$\begin{aligned} f &= (2\pi)^{3/2} \int_{\bar{\rho}_1=0}^1 \bar{\rho}_1^2 d\bar{\rho}_1 \int_{\cos \xi=-1}^1 d(\cos \xi) \left[1 + \varepsilon \frac{\sin \xi}{\bar{\rho}_1^{3/2} \sqrt{1-\bar{\rho}_1}} \right] \int_{\bar{\rho}_{12}=0}^{\rho_0} d\bar{\rho}_{12} \bar{F}(\mu_2) \\ &= (2\pi)^{3/2} \int_{\bar{\rho}_1=0}^1 d\bar{\rho}_1 \int_{\cos \xi=-1}^1 d(\cos \xi) \left[\bar{\rho}_1^2 + \varepsilon \sin \xi \sqrt{\frac{\bar{\rho}_1}{1-\bar{\rho}_1}} \right] \int_{\bar{\rho}_{12}=0}^{\rho_0} d\bar{\rho}_{12} \bar{F}(\mu_2) \end{aligned}$$

$$\bar{\rho}_1 \equiv \cos^2 \xi$$

$$y \equiv \cos \xi$$

$$z \equiv \frac{\bar{\rho}_{12}}{\rho_0}$$

$$x \equiv \frac{\bar{\rho}_2}{\rho_0}$$

$$\bar{\rho}_2^2 = \bar{\rho}_1^2 + \bar{\rho}_{12}^2 - 2\bar{\rho}_1 \bar{\rho}_{12} \cos \xi$$

$$x^2 = \left(\frac{\cos^2 \xi}{\rho_0} \right)^2 + z^2 - 2 \frac{\cos^2 \xi}{\rho_0} z y$$

$$x^2 = \bar{\varepsilon}^2 \cos^4 \xi + z^2 - 2 \bar{\varepsilon} z y \cos^2 \xi$$

$$f = (2\pi)^{3/2} \rho_0 \int_{\xi=0}^{\pi/2} 2 \cos \xi \sin \xi d\xi \int_{y=-1}^1 dy \left[\cos^4 \xi + \varepsilon \sqrt{1-y^2} \frac{\cos \xi}{\sin \xi} \right] \int_{z=0}^1 dz \bar{F}(\mu_2)$$

$$\mu_2 = \varepsilon_S \frac{z \rho_0 - x \rho_0}{z \rho_0 x \rho_0} = \frac{\bar{\varepsilon}^2}{\bar{\varepsilon}} \left(\frac{z-x}{xz} \right)$$

$$f = (2\pi)^{3/2} \rho_0 2 \int_{\xi=0}^{\pi/2} d\xi \cos^2 \xi \int_{y=-1}^1 dy \left[\cos^3 \xi \sin \xi + \varepsilon \sqrt{1-y^2} \right] \int_{z=0}^1 dz \bar{F}(\mu_2)$$

$$\frac{f(\varepsilon, \bar{\varepsilon}, \bar{\bar{\varepsilon}})}{2(2\pi)^{3/2} \rho_0} = \int_{\xi=0}^{\pi/2} d\xi \cos^2 \xi \int_{y=-1}^1 dy \left[\cos^3 \xi \sin \xi + \varepsilon \sqrt{1-y^2} \right] \int_{z=0}^1 dz \bar{F} \left(\bar{\varepsilon}^2 \frac{(z-x)/\bar{\varepsilon}}{xz} \right)$$

$$\bar{F}(\mu_2) = e^{\mu_2} \operatorname{erfc}(\sqrt{\max(0, \mu_2)}) \quad x^2 = \bar{\varepsilon}^2 \cos^4 \xi + z^2 - 2 \bar{\varepsilon} y z \cos^2 \xi$$

$$\varepsilon = \frac{\varepsilon_S^{3/2}}{r^2} \left(\frac{r_{ce}}{b} \right) \quad \bar{\varepsilon} = 1/\rho_0 \quad \bar{\bar{\varepsilon}} = \varepsilon_S^{1/2}/\rho_0$$

$$\bar{f}(\varepsilon, \bar{\varepsilon}, \bar{\bar{\varepsilon}}) \equiv \frac{f(\frac{1}{b}, \rho_0, \varepsilon_s)}{2(2\pi)^{3/2} \rho_0} \quad \Phi_b = \rho_0 \frac{e^{\varepsilon_s}}{\varepsilon_s^4} f(\varepsilon, \bar{\varepsilon}, \bar{\bar{\varepsilon}})$$

$$\Phi_b = \rho_0 \frac{e^{\varepsilon_s}}{\varepsilon_s^4} 2(2\pi)^{3/2} \rho_0 \bar{f}(\varepsilon, \bar{\varepsilon}, \bar{\bar{\varepsilon}})$$

$$\bar{g}(\bar{\varepsilon}, \bar{\bar{\varepsilon}}) \equiv \frac{g(\rho_0, \varepsilon_s)}{2(2\pi)^{3/2} \rho_0} = \int_{\xi=0}^{\pi/2} d\xi \sin \xi \cos^5 \xi \int_{y=-1}^1 dy \int_{z=0}^1 dz \bar{F}\left(\bar{\varepsilon}^2 \frac{(z-x)/\bar{\varepsilon}}{xz}\right)$$

$$\bar{h}(\bar{\varepsilon}, \bar{\bar{\varepsilon}}) \equiv \frac{h(\rho_0, \varepsilon_s)}{2(2\pi)^{3/2} \rho_0} = \int_{\xi=0}^{\pi/2} d\xi \cos^2 \xi \int_{y=-1}^1 dy \sqrt{1-y^2} \int_{z=0}^1 dz \bar{F}\left(\bar{\varepsilon}^2 \frac{(z-x)/\bar{\varepsilon}}{xz}\right)$$

so that

$$\bar{f}(\varepsilon, \bar{\varepsilon}, \bar{\bar{\varepsilon}}) = \bar{g}(\bar{\varepsilon}, \bar{\bar{\varepsilon}}) + \varepsilon \bar{h}(\bar{\varepsilon}, \bar{\bar{\varepsilon}})$$

and

$$\begin{aligned} \Phi_b &= \rho_0 \frac{e^{\varepsilon_s}}{\varepsilon_s^4} 2(2\pi)^{3/2} [\bar{g}(\bar{\varepsilon}, \bar{\bar{\varepsilon}}) + \varepsilon \bar{h}(\bar{\varepsilon}, \bar{\bar{\varepsilon}})] \\ &= \rho_0 \rho_0 [\bar{R}(\frac{1}{\rho_0}, \varepsilon_s) + (\frac{n_{ce}}{b}) \Delta \bar{R}(\frac{1}{\rho_0}, \varepsilon_s)] \equiv \Phi_z + \Phi_D \end{aligned}$$

$$\begin{aligned} \bar{R}_0(\frac{1}{\rho_0}) &= \min_{\varepsilon_s} (\bar{R}(\frac{1}{\rho_0}, \varepsilon_s)) \\ \min(\varepsilon_s) &= \varepsilon_{sm}(\frac{1}{\rho_0}) = \arg \min_{\varepsilon_s} (\bar{R}(\frac{1}{\rho_0}, \varepsilon_s)) \end{aligned}$$

$$\bar{R}_{OT}(\frac{1}{\rho_0}, \frac{n_{ce}}{b}) = \bar{R}_0(\frac{1}{\rho_0}) + (\frac{n_{ce}}{b}) \Delta \bar{R}_0(\frac{1}{\rho_0})$$

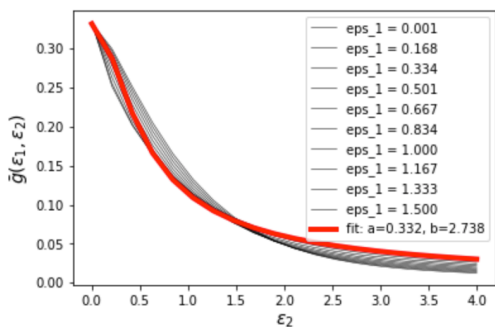
$$\Delta \bar{R}_0(\frac{1}{\rho_0}) = \Delta \bar{R}(\frac{1}{\rho_0}, \varepsilon_{sm})$$

$$\boxed{\begin{aligned} \Phi_b &= n^2 \bar{\omega} b^5 \rho_0 \bar{R}_{OT}(\frac{1}{\rho_0}, \frac{n_{ce}}{b}) \\ E_s &= k_B T_e \varepsilon_{sm}(\frac{1}{\rho_0}) \end{aligned}} \quad \begin{array}{l} \text{good value} \\ \text{is } \rho_0 = \frac{2}{3} \end{array}$$

$$\left. \begin{aligned} \Phi_b &\approx n^2 \bar{\omega} b^5 \left[\overbrace{(0.085)}^{\rho_0 \bar{R}_0(1/\rho_0)} + (2.5) \left(\frac{n_{ce}}{b} \right) \right] \\ E_s &\approx (4.5) k_B T_e \quad \overbrace{\rho_0 \Delta \bar{R}_0(1/\rho_0)} \end{aligned} \right\} \rho_0 = \frac{2}{3}$$

We will find that $\bar{g}$ is a very weak function of $\bar{\epsilon}$ so that $\bar{g}(\bar{\epsilon}, \bar{\epsilon}) \approx \bar{g}(\bar{\epsilon})$. We further will find that $\bar{g}(\bar{\epsilon}) \approx (1 + A^2 \bar{\epsilon}^2)^{-1/2/3}$. This now allows us to write

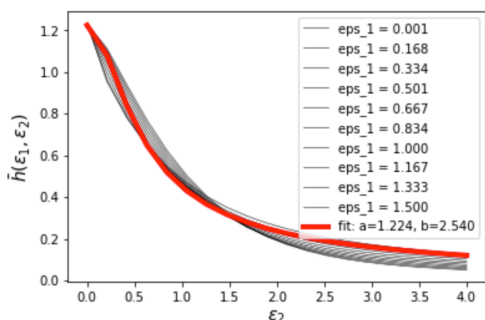
$$\Phi_z = R_0 \frac{e^{\epsilon_s}}{\epsilon_s^4} \frac{2(2\pi)^{3/2}}{3} \underbrace{\bar{g}\left(\frac{\epsilon_s^{1/2}}{\rho_0}\right)}$$



$$\approx \frac{1/3}{\sqrt{1 + A^2 \frac{\epsilon_s}{\rho_0^2}}} \quad A \approx 2.7$$

$$= R_0 \rho_0 \frac{e^{\epsilon_s}}{\epsilon_s^4} \frac{2(2\pi)^2}{3} (1 + A^2 \epsilon_s / \rho_0^2)^{-1/2}$$

$$\xrightarrow[\substack{1/\rho_0 \rightarrow 0 \\ \rho_0 \rightarrow \infty}]{} R_0 \rho_0 \frac{e^{\epsilon_s}}{\epsilon_s^4} \frac{2(2\pi)^2}{3} (\epsilon_s)_{\min} \rightarrow 4$$



$$\xrightarrow[\substack{\rho_0 \rightarrow 0 \\ 1/\rho_0 \rightarrow \infty}]{} R_0 \rho_0^2 \frac{e^{\epsilon_s}}{\epsilon_s^{4.5}} \frac{2(2\pi)^2}{3A} (\epsilon_s)_{\min} \rightarrow 4.5$$

We also find that $\bar{h}$ is a very weak function of $\bar{\epsilon}$. so that $\bar{h}(\bar{\epsilon}, \bar{\epsilon}) \approx \bar{h}(\bar{\epsilon})$. We further find that $\bar{h}(\bar{\epsilon}) \approx (1 + B^2 \bar{\epsilon}^2)^{-1/2} \frac{\pi^2}{8}$. Now

$$\Phi_0 = R_0 \rho_0 \frac{e^{\epsilon_s}}{\epsilon_s^{5/2}} \frac{2(2\pi)^{3/2}}{4\sqrt{2}} \left(\frac{r_{ce}}{b}\right) \bar{h}\left(\frac{\epsilon_s^{1/2}}{\rho_0}\right) \quad B \approx 2.5$$

$$= R_0 \rho_0 \frac{e^{\epsilon_s}}{\epsilon_s^{5/2}} \frac{(2\pi)^{3/2}}{4\sqrt{2}} \pi^2 \left(\frac{r_{ce}}{b}\right) (1 + B^2 \epsilon_s / \rho_0^2)^{-1/2}$$

$$\xrightarrow[\rho_0 \rightarrow \infty]{} R_0 \rho_0 \frac{e^{\epsilon_s}}{\epsilon_s^{2.5}} \frac{(2\pi)^{3/2}}{4\sqrt{2}} \pi^2 \left(\frac{r_{ce}}{b}\right) \quad \epsilon_{sm} \rightarrow 4$$

$$\xrightarrow[\rho_0 \rightarrow 0]{} R_0 \rho_0^2 \frac{e^{\epsilon_s}}{\epsilon_s^3} \frac{(2\pi)^{3/2}}{4\sqrt{2}} \frac{\pi^2}{B} \left(\frac{r_{ce}}{b}\right) \quad \epsilon_{sm} \rightarrow 4.5$$

Lets put a bound on $\bar{h}(\bar{\varepsilon}, \bar{\varepsilon})$ and Φ_0
 note that $\bar{F} \leq 1$ as before and do
 the integrals in expression for

$$\bar{h}(\bar{\varepsilon}, \bar{\varepsilon}) \leq \int_{\xi=0}^{\pi/2} d\xi \cos^2 \xi \int_{\theta=-\pi/2}^{\pi/2} d\theta \cos^2 \theta \quad \gamma = \sin \theta$$

$$\leq \left(\frac{\pi}{4}\right) \left(\frac{\pi}{2}\right) = \frac{\pi^2}{8}$$

$$\Phi_0 \leq R_0 \rho_0 \frac{e^{\varepsilon_s}}{\varepsilon_s^{5/2}} \frac{(2\pi)^{3/2}}{4\sqrt{2}} \pi^2 \left(\frac{r_{ce}}{b}\right) \text{ equality for } 1/\rho_0 = 0$$

$$\varepsilon_{sm} = 4 \Rightarrow (\Phi_0)_{\max} = R_0 \rho_0 \left(\frac{r_{ce}}{b}\right) \frac{e^4}{(4)^{2.5}} \frac{(2\pi)^{3/2}}{4\sqrt{2}} \pi^2$$

$$\approx (47) R_0 \rho_0 \frac{r_{ce}}{b}$$

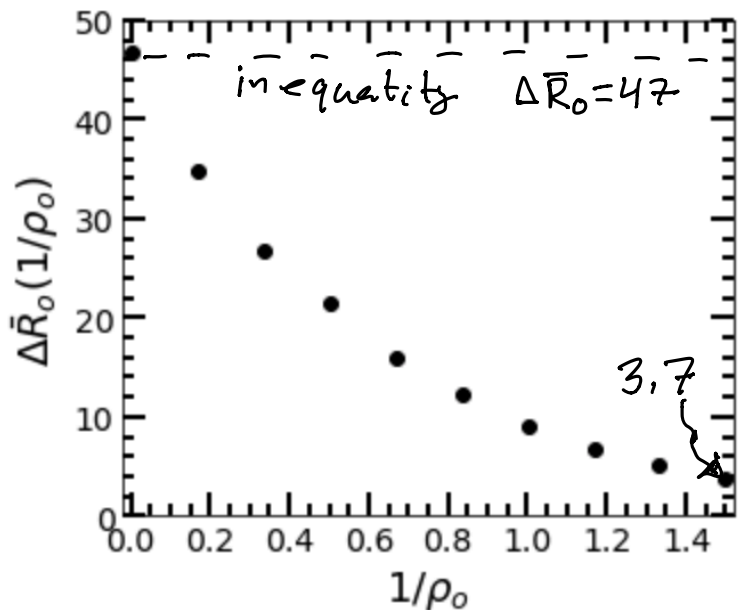
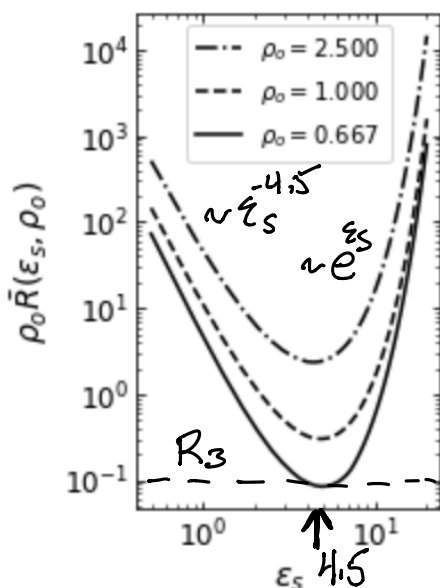
$$\Rightarrow \Phi_b \leq R_0 \rho_0 [(2.2) + (47)(r_{ce}/b)]$$

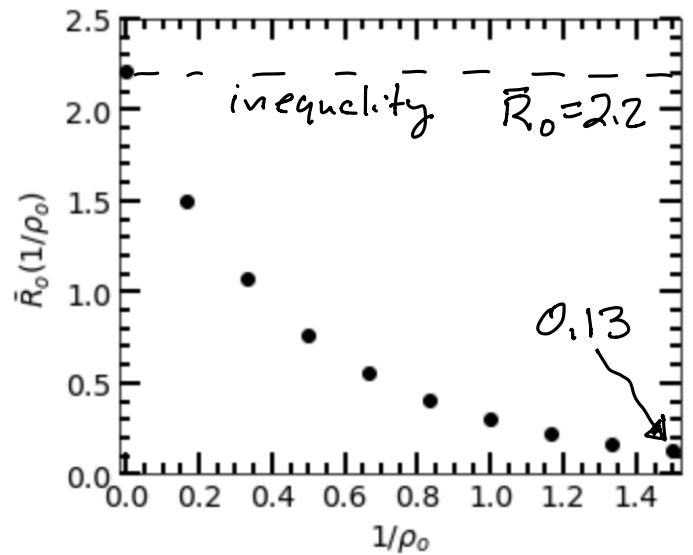
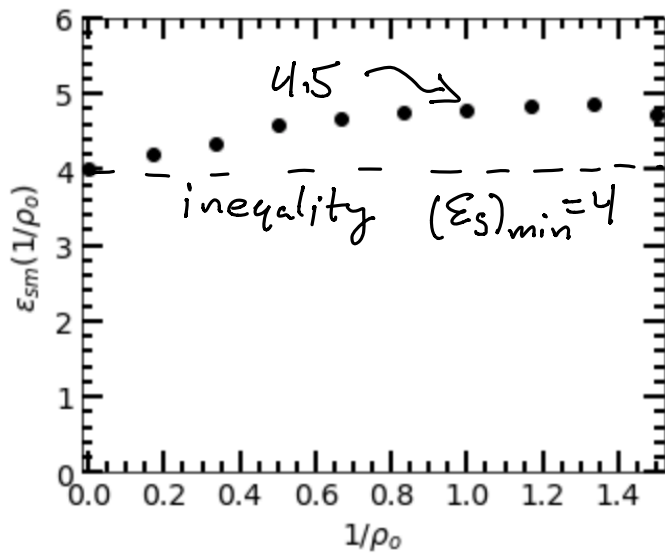
equality for $\rho_0 \rightarrow \infty$

$$\Phi_b = n^2 \bar{v} b^5 [(0.08) + (1.7)(r_{ce}/b)]$$

for $\rho_0 = 2/3$

Here is the more general dependance of
 $\Delta \bar{R}_0$





$$\bar{\Phi}_b = R_0 \rho_0 \left[\bar{R}_0\left(\frac{1}{\rho_0}\right) + \left(\frac{n_{ce}}{b}\right) \Delta \bar{R}_0\left(\frac{1}{\rho_0}\right) \right] = \bar{\Phi}_z + \bar{\Phi}_D$$

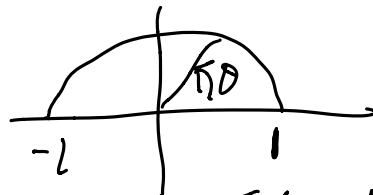
$$@ \rho_0 = 2/3$$

$$\bar{\Phi}_b = n^2 \bar{v} b^5 \left[(0.085) + \left(\frac{n_{ce}}{b}\right) (2.5) \right]$$

Calculation of $G(c)$

$$\sin \theta_0 = \frac{1}{\sqrt{1+c^2}}$$

$$\cos \theta_0 = \frac{-c}{\sqrt{1+c^2}}$$



$$\cos \theta = 1$$

$$d(\cos \theta) [\cos \theta + C \sin \theta]$$

$$\pi \leq \theta \leq 0$$

$$-1 \leq \cos \theta \leq 1$$

$$\cos \theta = \cos \theta_0$$

$$\theta_0 = \cos^{-1} \frac{-c}{\sqrt{1+c^2}}$$

$$0 \leq \cos^{-1} \leq \pi$$

$$\theta = \theta_0$$

$$= \int_{\theta_0}^{\theta_0} d\theta [\sin \theta \cos \theta + C \sin^2 \theta]$$

$$= \int_0^{\theta_0} d\theta \sin \theta \cos \theta + C \int_0^{\theta_0} d\theta \sin^2 \theta$$

$$= \int_{\cos \theta_0}^1 d(\cos \theta) \cos \theta + C \int_0^{\theta_0} d\theta \left[\frac{1}{2} - \frac{1}{2} \cos(2\theta) \right]$$

$$= \left| \frac{\cos^2 \theta}{2} \right|_{\cos \theta_0}^1 + C \left| \frac{\theta}{2} - \frac{1}{4} \sin 2\theta \right|_0^{\theta_0}$$

$$= \left(\frac{1}{2} - \frac{\cos^2 \theta_0}{2} \right) + C \left[\frac{\theta_0}{2} - \frac{1}{4} \sin 2\theta_0 \right]$$

$$\frac{1}{2} \sin \theta_0 \cos \theta_0$$

$$\left. \begin{aligned} \sin(\alpha + \beta) &= \sin \alpha \cos \beta + \sin \beta \cos \alpha \\ \sin 2\alpha &= 2 \sin \alpha \cos \alpha \\ \cos(\alpha + \beta) &= \cos \alpha \cos \beta - \sin \alpha \sin \beta \end{aligned} \right\}$$

$$\begin{aligned}
 \cos 2\theta &= \cos^2 \theta - \sin^2 \theta \\
 &= 1 - \sin^2 \theta - \sin^2 \theta \\
 &= 1 - 2\sin^2 \theta \\
 \therefore \sin^2 \theta &= \frac{1}{2}(1 - \cos 2\theta) \\
 &= \frac{1}{2} \left(1 + C \frac{\theta_0}{2} \right) - \frac{1}{2} \left(\cos^2 \theta_0 + C \sin \theta_0 \cos \theta_0 \right) \\
 &= \frac{1}{2} \left(1 + C \frac{\theta_0}{2} \right) \quad \underbrace{\frac{c^2}{1+c^2} + C \frac{-c}{1+c^2}}_{\emptyset}
 \end{aligned}$$

$$\begin{aligned}
 &= \frac{1}{2} \left[1 + C \cos^{-1} \left(\frac{-c}{\sqrt{1+c^2}} \right) \right] \quad (0 \leq \cos^{-1} x \leq \pi) \\
 &= \frac{1}{2} \left[1 + C \cot^{-1}(-c) \right] \quad (0 \leq \cot^{-1} x \leq \pi)
 \end{aligned}$$

Calculation of $\bar{G}(a)$

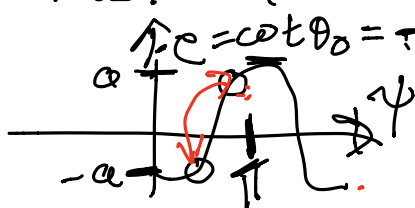
$$C = a \cos \psi$$

$$\cot^{-1}(-C) = \theta_0 \quad -c = \cot \theta_0 \quad \theta_0 \text{ gives } \theta_0(\psi)$$

$$C = -\cot \theta_0 = a \cos \psi$$

$$\begin{aligned}
 \int_0^{2\pi} G(C(\psi)) d\psi &= \int_0^{2\pi} \frac{1}{2} [1 + C \cot^{-1}(-c)] d\psi = \int_0^{2\pi} \frac{1}{2} [1 - \theta_0 \cot \theta_0] d\psi \\
 &= \bar{G}(a) \quad \text{where } \theta_0(\psi)
 \end{aligned}$$

$$\begin{aligned}
 \psi &: 0 \rightarrow \frac{\pi}{2} \rightarrow \pi \rightarrow \frac{3\pi}{2} \rightarrow 2\pi \\
 a \cos \psi &: a \rightarrow 0 \rightarrow -a \rightarrow 0 \rightarrow a \\
 \uparrow C = \cot \theta_0 &= -a \cos \psi
 \end{aligned}$$



$$\cot \psi = -\cot(\pi - \psi)$$

$$\pi - \cot^{-1}(-c) = \cot^{-1}(c)$$

$$\begin{aligned} \frac{1}{2} \int_0^{2\pi} \theta_0 \cot \theta_0 d\psi &= \int_0^{\pi/2} \theta_0 \cot \theta_0 d\psi - \int_0^{\pi/2} (\pi - \theta_0) \cot \theta_0 d\psi \\ &= \pi \int_0^{\pi/2} \cot \theta_0 d\psi = -a\pi \int_0^{\pi/2} \cos \psi d\psi = -a\pi \end{aligned}$$

$\cot \theta_0 = -\cot(\pi - \theta_0)$
 negative direction
 $\int_0^{\pi/2} -\cot$

$$\begin{aligned} \Rightarrow \frac{1}{2} \int_0^{2\pi} (1 - \theta_0 \cot \theta_0) d\psi \\ = \frac{1}{2} \int_0^{2\pi} (1 + 2\pi a \cos \psi) d\psi \\ = \frac{1}{2} (2\pi + 2\pi a) \\ = \pi(1+a) = \bar{G}(a) \end{aligned}$$