Three-body Recombination in a Strong Magnetic Field

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[M. E. Glinsky and T. M. O'Neil, Bul. Am. Phys. Soc. **34**, 1934 (1989)]

Abstract*

We say that a bound electron-proton system is a guiding center atom when the electron motion is classical and can be treated with guiding center dynamics. The cyclotron radius for the electron must be small compared to the electron-proton separation. Such atoms are expected to occur during the initial phase of recombination, when a proton is introduced into a strongly magnetized and cryogenic electron plasma.[1] This paper discusses the three-body recombination process that produces such atoms. Equations describing the evolution in the state of the guiding center atom are derived from the BBGKY hierachy for a guiding center electron plasma. These equations are examined analytically and simulated numerically using a Monte Carlo method. The recombination rate and other details of the recombination cascade to deeper binding are obtained.

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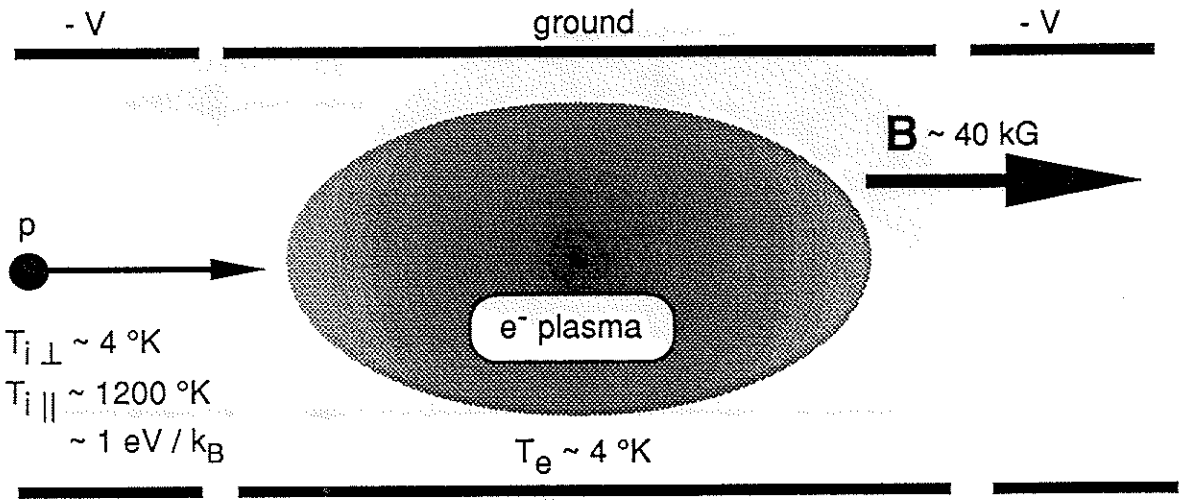
[1]B. Beck, J. Fajans and J. Malmberg, Bull. Am. Phys. Soc. **33** 2004 (1988).

Basic System

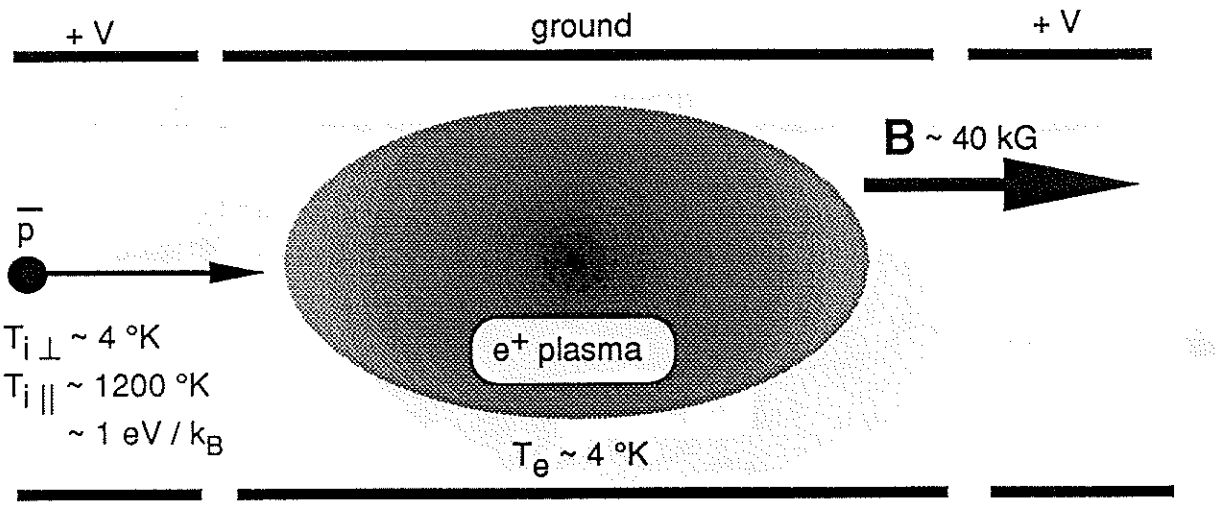


How fast and by what mechanism will a proton and an electron recombine into hydrogen?

Reference

J.H. Malmberg, T. M. O'Neil, A.W. Hyatt and C.F. Driscoll, "The Cryogenic Pure Electron Plasma", *Proc. of 1984 Sendai Symposium on Plasma Nonlinear Phenomena*, 31 (1984).

Anti-matter Analogue



How fast and by what mechanism will an antiproton and a positron recombine into antihydrogen?

References

- **Positron Trap**

  C.M. Surko et. al., Rev. Sci. Instr. **57** , 1862 (1986).
  C.M. Surko, M. Leventhal and A. Passner, Phys. Rev. Lett. **62**, 901 (1989).

- **Antiproton Trap**

  G. Gabrielse et. al., Phys. Rev. Lett. **57**, 2504 (1986).

  X. Fei, R. Davisson and G. Gabrielse, Rev. Sci. Instr. **58**, 2197 (1987).

- **Antihydrogen Production**

  G. Gabrielse, S. L. Rolston, L. Haarsma and W. Kells, Phys. Lett. **A129**, 38 (1988).

- **Spectroscopy and Gravitation Study of Trapped Antihydrogen**

  G. Gabrielse, "Trapped Antihydrogen for Spectroscopy and Gravitation Studies: Is It Possible?", *Proc. of the Symposium on the Production and Investigation of Atomic Antimatter* , edited by H. Poth and A. Wolf (Scientific, Basel, 1988).

Parameter Regime

$$n b^3 << 1$$

(weakly correlated)

$$\frac{r_c}{b} << 1$$

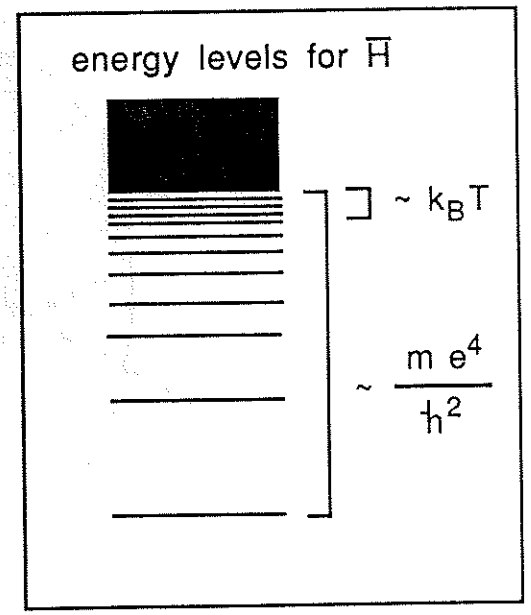
(guiding center dynamics)

$$\frac{\bar{v}_{i\perp}}{\bar{v}_e} << \frac{r_c}{b}$$

(small $\perp$ ion velocity)

$$\lambda_t << b \quad \text{or} \quad k_B T << \frac{m e^4}{2\hbar^2} \approx 13\ \text{eV}$$

(classical dynamics)



where

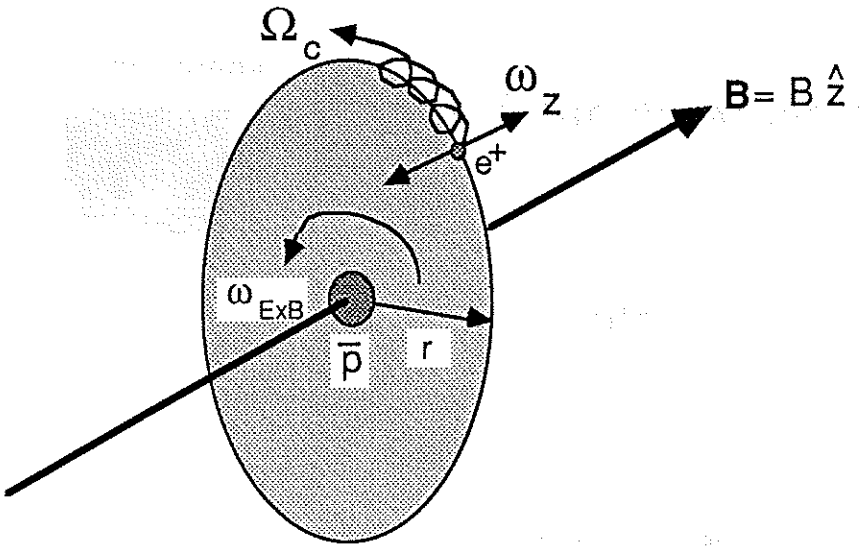
$b = \frac{e^2}{k_B T}$ = distance of closest approach

$r_c = \frac{\bar{v}_e}{\Omega_c}$ = cyclotron radius

$\Omega_c = \frac{e B}{m_e c}$ = cyclotron frequency

$\lambda_t = \frac{h}{m \bar{v}_e}$ = thermal de Broglie wavelength

Guiding Center Dynamics



Ordering of Frequencies

$$\Omega_c >> \omega_z >> \omega_{E\times B} >> \frac{\overline{v}_{i\perp}}{r}$$

Collisional 3-Body Recombination Dominates at Low Temperatures

$$\text{Rate}_{\text{3-body recombination}} \sim \underbrace{\left(n \bar{v}_e b^2\right)}_{\text{rate of collision}} \cdot \underbrace{\left(n b^3\right)}_{\substack{\text{probability another positron close enough to carry away momentum}}}$$

$$\sim \omega_{pe} \left(n b^3\right)^{3/2}$$

$$\sim \omega_{pe} \left(\frac{n^{1/3} e^2}{k_B T}\right)^{9/2}$$

At low temperatures the temperature scaling of this rate ($T^{-9/2}$) makes 3-body recombination the dominant process.

Monte Carlo Calculation of Rates

For B=0,
the calculation by Mansbach and Keck shows

$$\text{Rate} \approx 0.76(4)\ n^2 b^5 \bar{v}_e$$

[P. Mansbach and J. Keck, Phys. Rev. **181**, 275 (1969).]
[B. Makin and P. Mansbach, Phys. Rev. Lett. **11**, 281 (1963).]

For $r_c << b$,
we have calculated

$$\text{Rate} \approx 0.070(10)\ n^2 b^5 \bar{v}_e$$

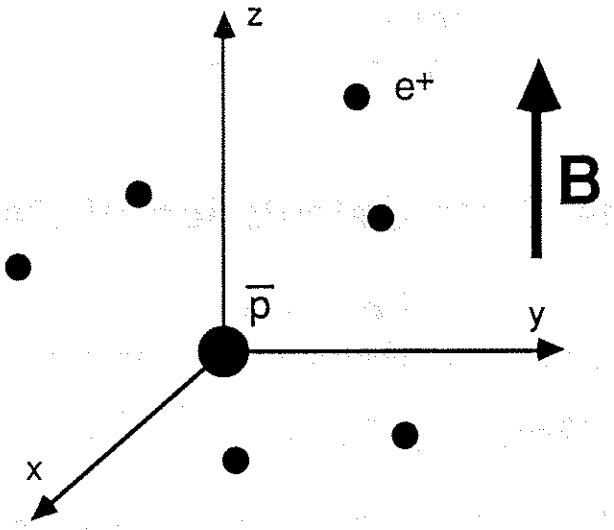
Theoretical Framework

Consider ensemble of

(1) fixed $\bar{\mathbf{p}}$ at origin
(2) N positrons undergoing guiding center dynamics

with boundary conditions

(1) thermal equilibrium at large distance from $\bar{\mathbf{p}}$
(2) positrons which reach deep binding are removed and returned to the distant plasma

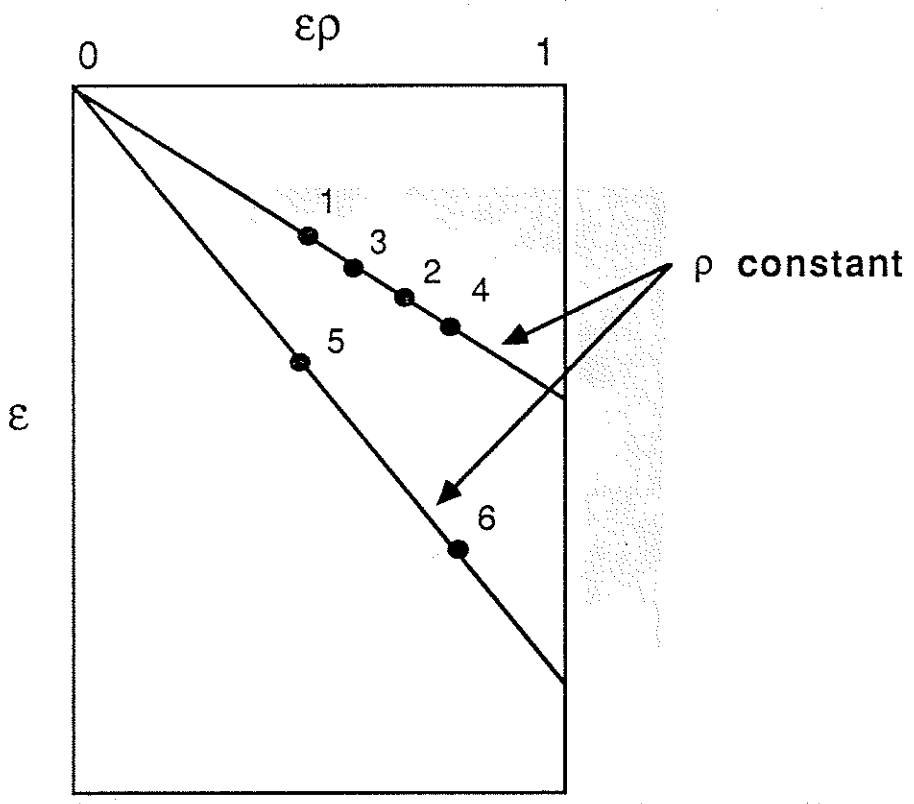


$R_{3\text{-body}}$ = steady state flux to deep binding

State of Guiding Center Atom

For convenience we use $f_1(\varepsilon,\varepsilon\rho)$ where

$$\varepsilon \equiv \frac{-\left(\frac{p_z^{\,2}}{2\,m_e} - \frac{e^2}{\sqrt{z^2+r^2}}\right)}{k_B\,T} \qquad \varepsilon\rho \equiv \varepsilon\,\frac{r}{b}$$



Boundary Conditions

As $\varepsilon \to 0$ $\quad f / f_{eq} \to 1$

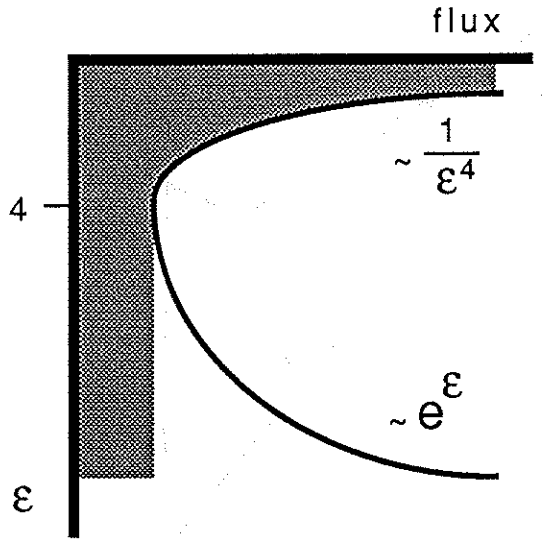
As $\varepsilon \to \infty$ $\quad f / f_{eq} \to 0$

Bottleneck

The one way thermal equilibrium flux through an ε=constant surface scales as

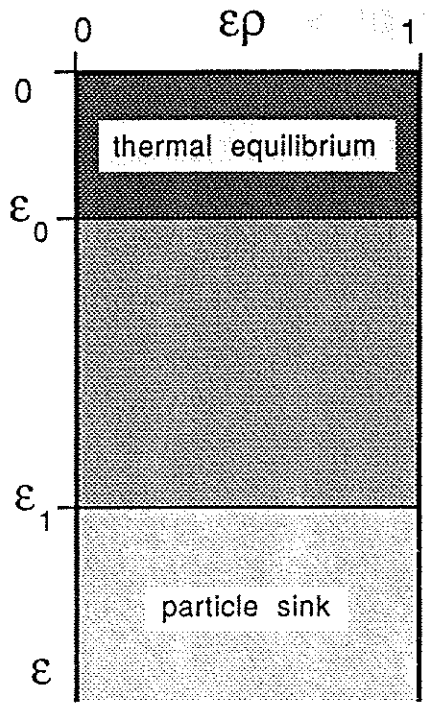
$$\text{flux} \sim \frac{e^{\varepsilon}}{\varepsilon^{4}}$$

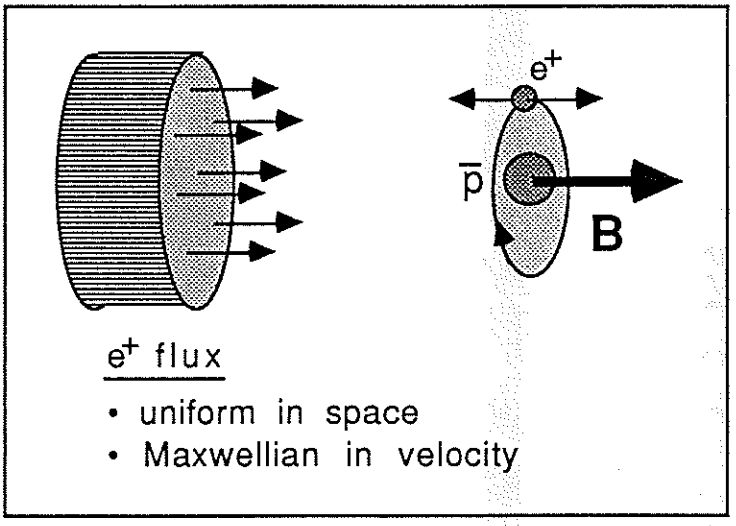
dominated by the phase space factor, $1/\varepsilon^{3.5}$, and the Boltzmann factor, e^{ε}. This flux has a strong minimum at ε=4.



In steady state, the rate through any ε surface will be a constant. It is obvious that this rate can not be larger than the minimum flux through an ε=constant surface. Therefore, the distribution function for states above the bottleneck will nearly attain its thermal equilibrium value and below the flux minimum the distribution function will be significantly less than its equilibrium value. This is in close analogy with water flowing through the neck of a bottle, hence the name bottleneck.

Monte Carlo Code





Numerical algorithm is:

• Pick state of guiding center atom in thermal distribution. Collide a positron from Maxwellian flux. Repeat these steps until an atom with energy below ε_0 is formed.

• Once formed, continue to collide positrons with the guiding center atom. This will trace out a trajectory in $(\varepsilon,\varepsilon\rho)$ space. Do this until the state of the atom crosses ε_0 or ε_1.

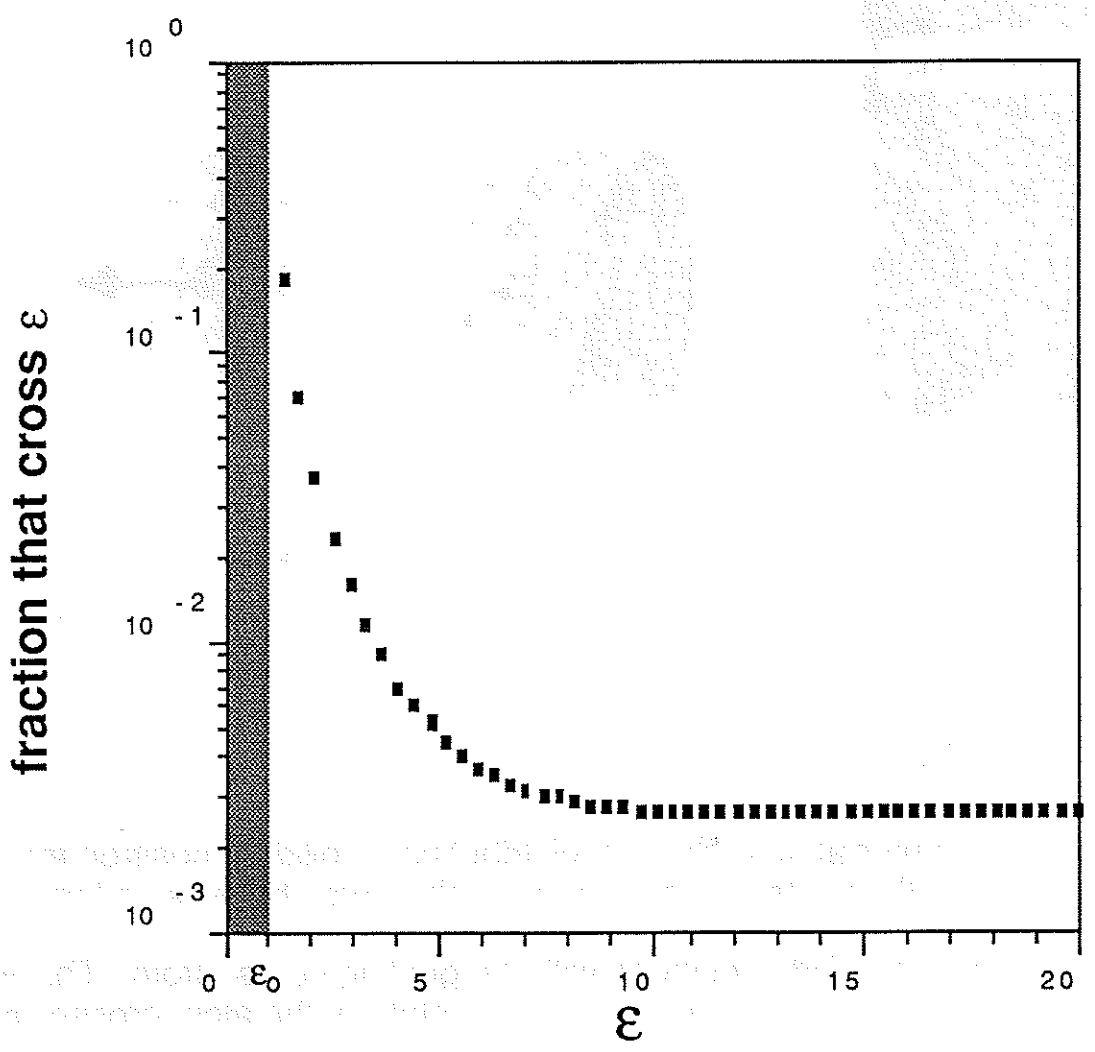
The recombination rate will be

$$\text{Rate}_{\text{recombine}} = \frac{1}{\left\langle \text{time for formation of atom which crosses } \varepsilon_1 \right\rangle}$$

and the steady state distribution, $f_{ss}(\varepsilon,\varepsilon\rho)$, in the area between ε_0 and ε_1 will be proportional to the amount of time spent in a $\Delta\varepsilon\Delta\varepsilon\rho$ box at $(\varepsilon,\varepsilon\rho)$ divided by $\Delta\varepsilon\Delta\varepsilon\rho$.

Bottleneck Exists

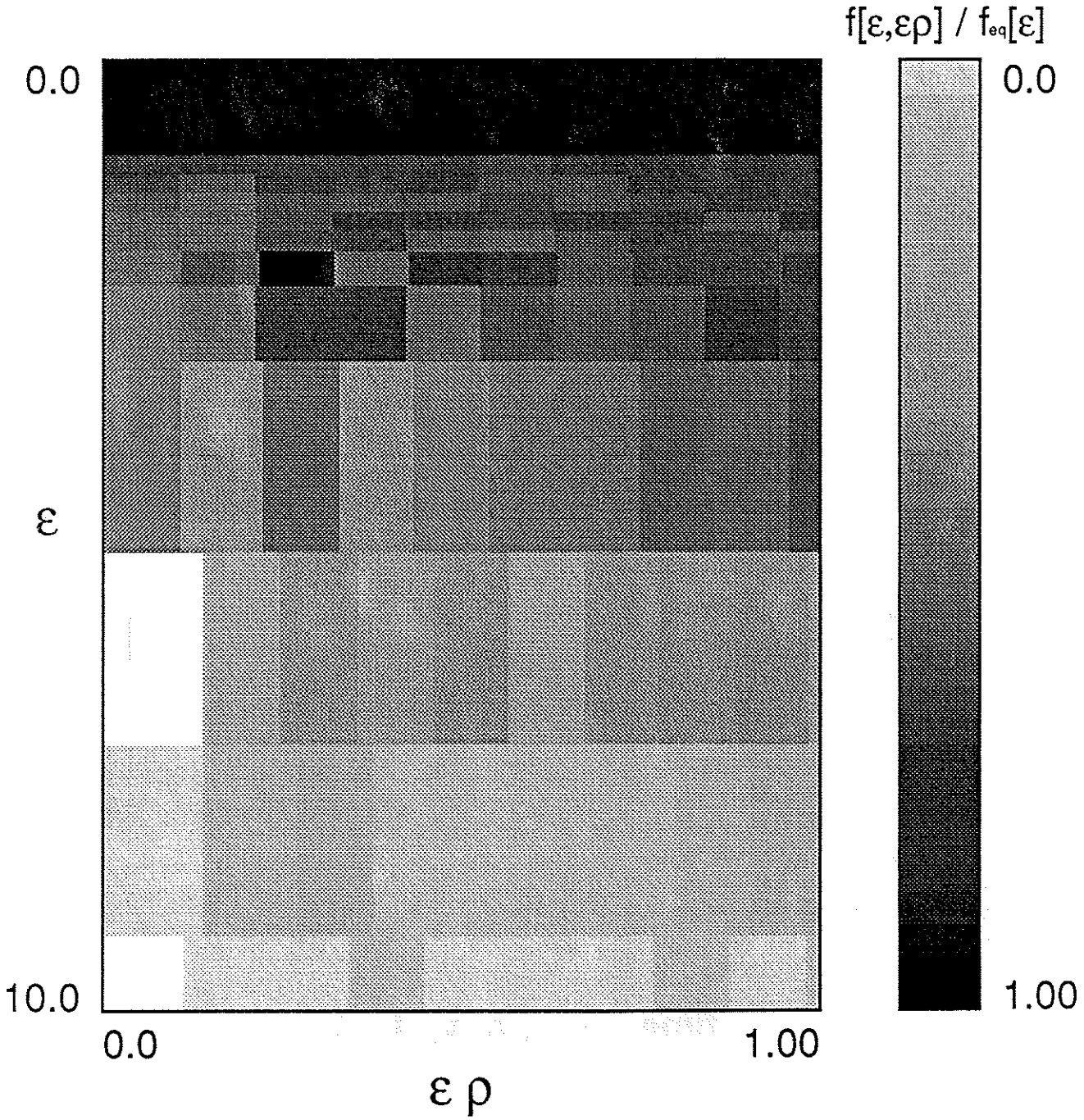
Fraction of Atoms Initially Formed (ε_o =1) that Make it to States with Energy > ε .



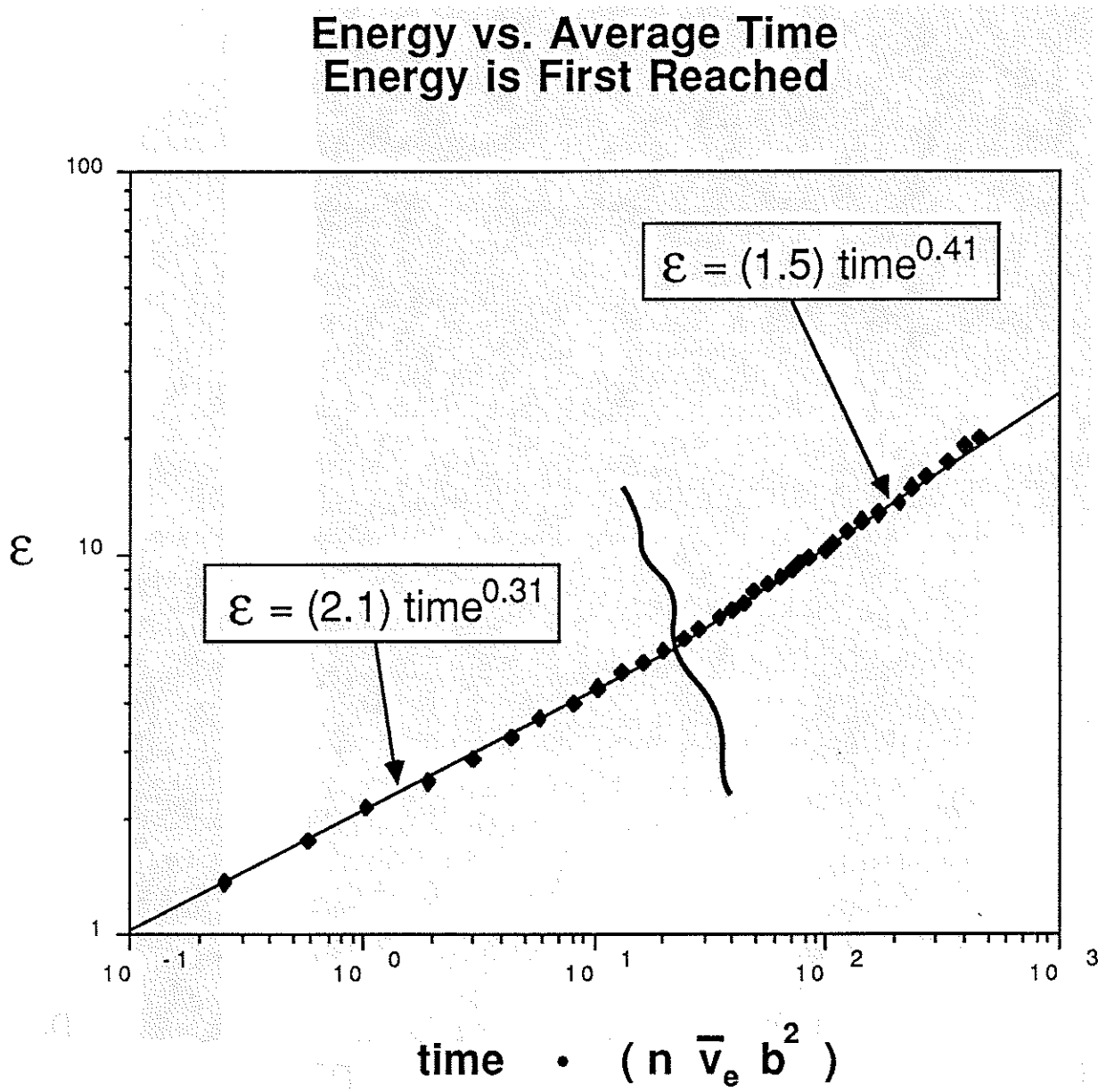
If a bound positron makes it to a state below the bottleneck of $\varepsilon \approx 5$, then it continues to be more bound. This makes it possible to unambiguously define a recombination. The rate for such recombinations is

$$\text{Rate}_{\text{Recombination}} = 0.070(10)\ n^2 b^5 \overline{v}_e$$

Steady State Distribution



Time to Capture Positron



Scaling of Time to Capture

Assume that the rate of collision of a positron with the atom is proportional to the area within an adiabatic cutoff

$$\text{Rate} \sim r_{\text{cutoff}}^2$$

The cutoff for small ε is the radius for which

$$\frac{r_{\text{cutoff}}}{\bar{v}_e}\,\omega_z \sim 1 \quad \Rightarrow \quad \frac{r_{\text{cutoff}}}{b} \sim \frac{1}{\varepsilon^{3/2}}$$

For large ε the above cutoff gets much smaller than the average separation of the positron from the antiproton,

$$\frac{< r >}{b} \sim \frac{1}{\varepsilon}$$

Therefore, for large ε, $< r >$ must be used in place of r_{cutoff} to determine the rate.

From the numerics the scaling of the average step size has been found to be

$$< \Delta\varepsilon > \sim \varepsilon$$

Now

$$\frac{d\varepsilon}{dt} = \frac{\Delta\varepsilon}{\Delta t} = (\text{Rate})\,(\Delta\varepsilon) \sim \frac{1}{\varepsilon^2} \quad \text{(small } \varepsilon\text{)}$$

$$\sim \frac{1}{\varepsilon} \quad \text{(large } \varepsilon\text{)}$$

Whose solution is

$$\varepsilon(t) \sim t^{1/3} \quad \text{(small } \varepsilon\text{)}$$

$$\sim t^{1/2} \quad \text{(large } \varepsilon\text{)}$$

Integration of Ion-Electron System

By a series of canonical transformations the Hamiltonian for an ion (full dynamics) and an electron (guiding center dynamics) can be written as

$$H(R, J_z; \psi, p_\psi) =$$

$$\Omega_i\left(p_\psi - R\sqrt{2 m_e \Omega_e p_\psi}\cos\psi\right) + H_1(J_z, p_\psi)$$

$$R, J_z \text{ constant}$$

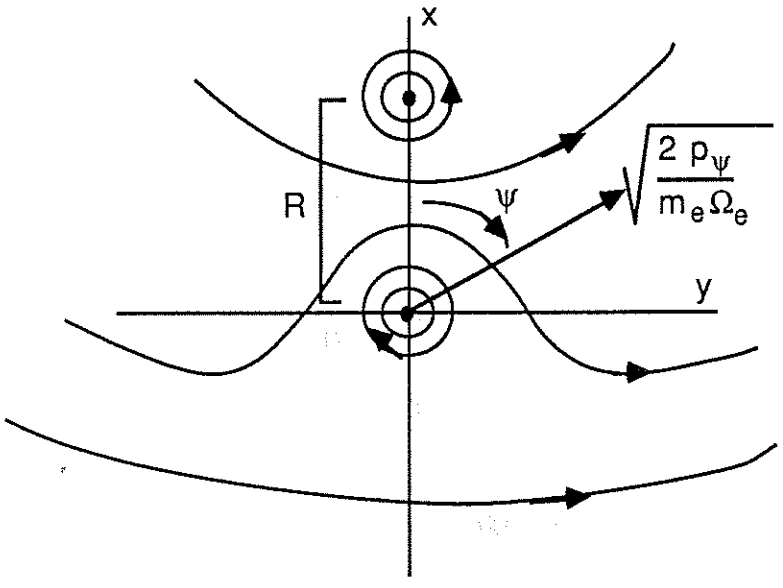
where

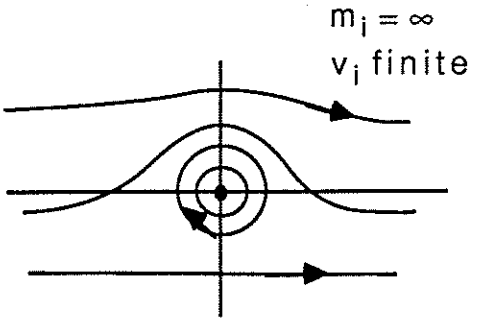
$$\vec{R} = \left[(\vec{r}_i)_\perp + \frac{m_e c}{e}\frac{\vec{v}_i \times \vec{B}}{B^2}\right] - (\vec{r}_e)_\perp$$

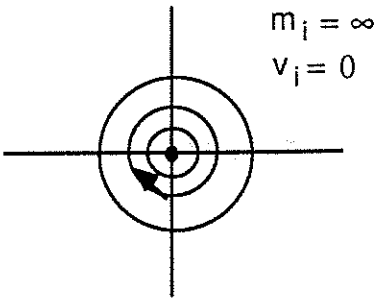
$$\left|(\vec{r}_i - \vec{r}_e)_\perp\right| = \sqrt{\frac{2 p_\psi}{m_e \Omega_e}}$$

$$\psi = \angle\left(\vec{R}, (\vec{r}_i - \vec{r}_e)_\perp\right)$$

It has been assumed that $\omega_z >> \omega_{E\times B}$.







Further Work

If $\bar{v}_i$ is finite, then

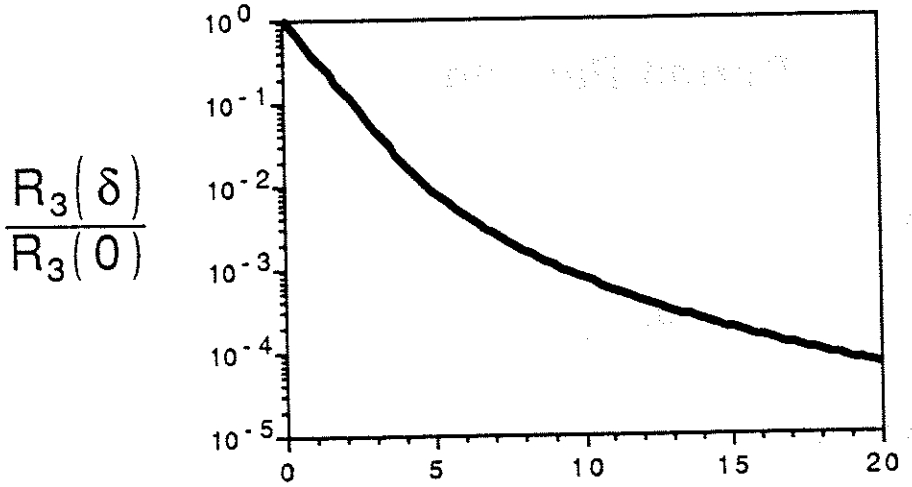
$$n_e \bar{v}_e b^2 << \omega_{ExB}$$

$$m_i = 0$$

is the worst case because the ion can run away to infinity before the next collision.

We will simulate this case.

Expect $f_1(J_z, J_\Omega)$ to equal a constant (not be proportional to e^{ε}) outside the separatrix. This leads to the following prediction for the three-body recombination rate.



$$\delta = \sqrt{\frac{v_i / b}{\omega_{ExB}}}$$

Transport Equation

Evolution is governed by the Liouville equation. Partial integration of this equation yields the BBGKY Hierarchy.

1-Particle Equation

Let $f_1 = f_1(z_1, r_1, E_1; t)$ since by symmetry $\partial f_1 / \partial \theta_1 = 0$

$$\frac{\partial f_1}{\partial t} + v_1 \frac{\partial f_1}{\partial z_1}\bigg)_{E_1} = n \int d\vec{x}_2 \, dv_2 \, \frac{\partial}{\partial z_1}\left(\frac{e^2}{|\vec{x}_1 - \vec{x}_2|}\right) v_1 \frac{\partial f_2(1,2)}{\partial E_1}$$

Due to the fact that $\frac{\bar{v}_e}{b} >> \bar{v}_e \, b^2 \, n_e \quad (n_e \, b^3 << 1)$ the distribution function relaxes to

$$f_1 = f_1^{(0)}(E_1, r_1; t) + f_1^{(1)}(z_1, E_1, r_1; t)$$

Unbound Particles

$$f_1^{(0)}(E_1, r_1; t) = \sqrt{\frac{m_e}{2 \pi k_B T_e}} \, e^{-E_1 / k_B T_e} = f_B(E_1)$$

Bound Particles

Define

$$W(E_1, r_1; t) = n \oint_{E_1} \frac{dz_1}{m_e v_1} f_1^{(0)}(E_1, r_1; t)$$

where $dN = 2 \pi r_1 \, W(E_1, r_1; t) \, dE_1 \, dr_1$

The evolution is given by

$$\frac{\partial W}{\partial t} = \frac{\partial}{\partial E_1}\left\{ n^2 \oint \frac{dz_1}{m_e v_1} \int d\vec{x}_2 \, dv_2 \, \frac{\partial}{\partial z_1}\left(\frac{e^2}{|\vec{x}_1 - \vec{x}_2|}\right) v_1 \, f_2(1,2) \right\}$$

Diffusion Calculation

Consider the effect of large impact parameter collisions

$$|\vec{x}_2| \geq d_c >> |\vec{x}_1|$$

Solve for f_2 to 1st order in $1/|x_2|$.

$$f_2 = f_2^{(0)} + \delta f_2 \qquad f_2^{(0)}(1,2) = f_1^{(0)}(1)\, f_1^{(0)}(2)$$

2-Particle Equation

$$\left\{ \frac{\partial}{\partial t} + v_1 \frac{\partial}{\partial z_1}\Big)_{E_1} + v_2 \frac{\partial}{\partial z_2}\Big)_{E_2} - \frac{\partial}{\partial z_1}\left(\frac{e^2}{|\vec{x}_1 - \vec{x}_2|} \right)\left[v_1 \frac{\partial}{\partial E_1} - v_2 \frac{\partial}{\partial E_2} \right] \right\} f_2(1,2) \approx 0$$

which neglects close 3-particle collisions since $(n\, b^3 << 1)$.

Integration of this equation along the unperturbed orbits

$$z_2(t') = z_2 + v_2(t' - t) \qquad v'_2 = v_2$$

$$z_1(t') = a_1 \cos\left[\omega_1 (t' - t) + \psi_1 \right]$$

$$\omega_1^2 = \frac{e^2}{m_e r_1^3} \qquad E_1 = -\frac{e^2}{r_1} + \frac{m_e \omega_1^2 a_1^2}{2}$$

(for simplicity we have assumed deep binding) yields

$$\delta f_2 = \int_{-\infty}^{t} dt' \left[\frac{\partial}{\partial z_1}\left(\frac{e^2}{|\vec{x}_1 - \vec{x}_2|} \right) \right]' \left(v'_1 \frac{\partial}{\partial E_1} - v'_2 \frac{\partial}{\partial E_2} \right) f_2^{(0)}$$

Substitution into the 1-particle equation yields

$$\frac{\partial W(E_1, r_1, t)}{\partial t} = \frac{\partial}{\partial E_1}\left\{ D_{\|}(E_1, r_1)\, n\left[\frac{1}{k_B T_e}\, f_1^{(0)}(E_1, r_1) + \frac{\partial f_1^{(0)}(E_1, r_1)}{\partial E_1} \right] \right\}$$

where

$$D_{\|}(E_1, r_1) = (k_B T_e)^2 \left(n_e b^2 \bar{v}_e\right)\left(\frac{a_1 \omega_1}{\bar{v}_e}\right)^2 \frac{2\pi}{m_e \omega_1}\sqrt{8\pi}\quad I(\alpha)$$

$$\alpha = \frac{d_c \omega_1}{\bar{v}_e}$$

$$I(\alpha) = \int_0^{\infty} \frac{dx}{x}\, e^{-x^2/2} \int_{\alpha/x}^{\infty} d\xi\; \xi\; K_0^2(\xi)$$

Note the:

(1) adiabatic cutoff for large d_c (i.e., large α)

$$I(\alpha) \sim e^{-\frac{3}{\sqrt[3]{2}}\alpha^{2/3}}\, \alpha^{-1/3}$$

(2) importance of small impact parameter collisions.

If we had retained **E**×**B** drift motion we would have obtained

$$D = D_{\|} + D_{\perp}$$

where

$$D_{\perp} \sim \left(\frac{r_{ce}}{b}\right)^2 D_{\|}$$

Variational Theory of Reaction Rates

Let's calculate the 1-way thermal equilibrium flux though the surface $E_1 = E_\sigma$.

$$R_\sigma = n^2 \int_{E_1 = E_\sigma} 2\pi\, r_1\, dr_1\, d\vec{x}_2\, dv_2\, \frac{\partial}{\partial z_1}\left(\frac{e^2/m_e}{|\vec{x}_1 - \vec{x}_2|}\right) f_2(1,2)$$

$$\frac{dE_1}{dt} = -v_1 \frac{\partial}{\partial z_1}\left(\frac{e^2}{|\vec{x}_1 - \vec{x}_2|}\right) > 0$$

adiabatic cutoff $r_{cut} = \frac{\rho_0}{\varepsilon} b$ is imposed

where

$$f_2(1,2) = \frac{m_e}{2\pi k_B T_e} \exp\left(-\frac{1}{k_B T_e}\left[E_1 + E_2 + \frac{e^2}{|\vec{x}_1 - \vec{x}_2|}\right]\right)$$

This integral can be approximated as

$$R_\sigma = n^2 \bar{v}_e b^5 \frac{2(2\pi)^{3/2}}{3} \frac{e^{\varepsilon_\sigma}}{\varepsilon_\sigma^4} \rho_0$$

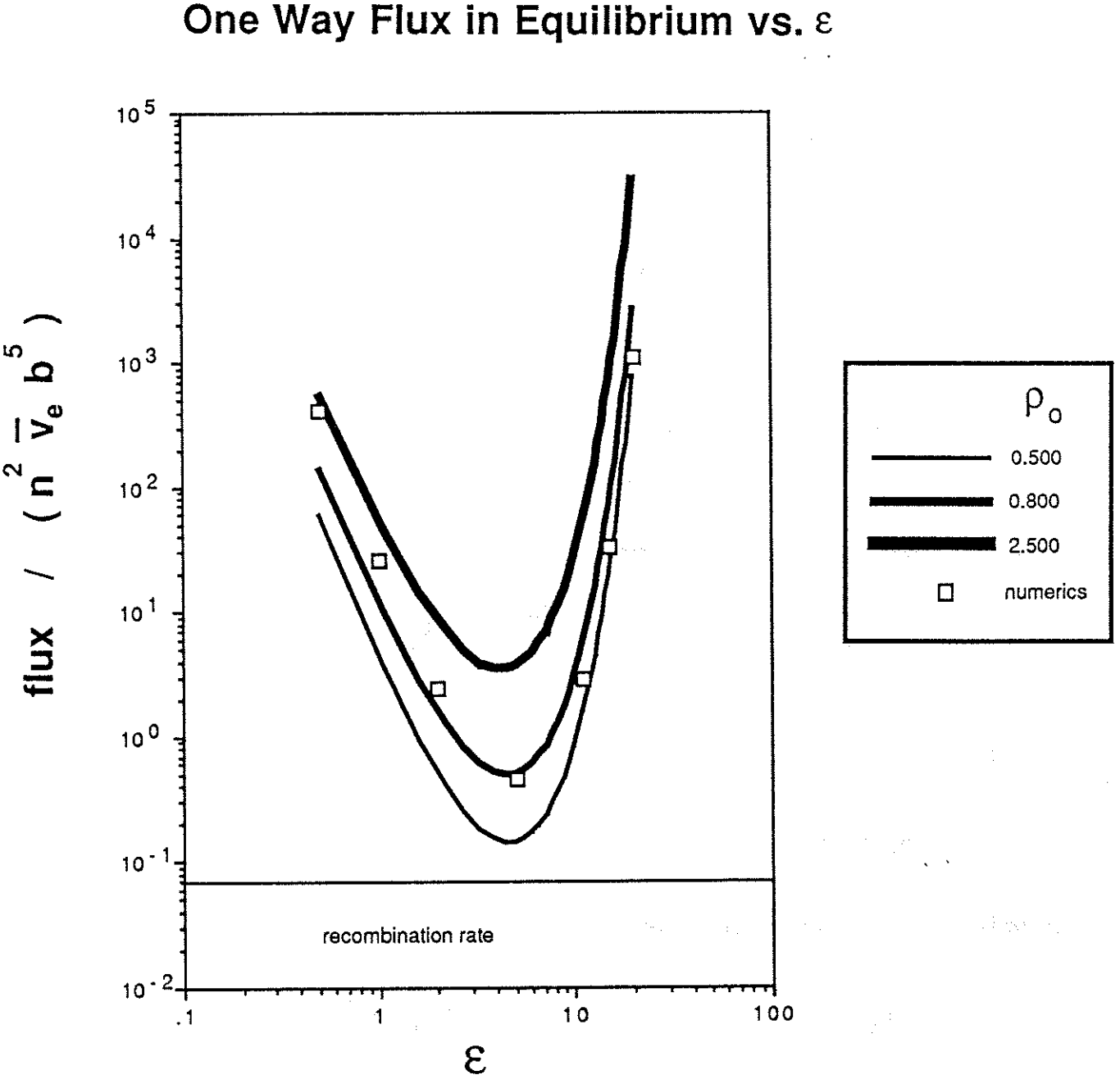
where $\varepsilon_\sigma = -E_\sigma / k_B T_e$

R_σ has a minimum at $\varepsilon_\sigma = 4$.

The variational theory assumes

$$R_3 = R_\sigma(\varepsilon_\sigma = 4) = 2.2\, n^2 \bar{v}_e b^5 \rho_0$$

Comparison of Monte Carlo Code's Equilibrium One Way Flux to the Analytically Calculated Flux.



Master Equation

Operating on the 2-particle equation with $\oint_{E_1} \frac{dz_1}{m_e v_1} \int d\vec{x}_2\, dv_2$ and substitution of the result into the 1-particle equation yields

$$\frac{\partial W(E_1, r_1; t)}{\partial t} = n^2 \oint_{E_1} \frac{dz_1}{m_e v_1} \int d\vec{x}_{2\perp}\, dv_2\, v_2 \left[f_2(z_2 = +\infty) - f_2(z_2 = -\infty) \right]$$

Now we set

$$f_2(z_2 = -\infty) = f_1^{(0)}(E_1, r_1; t)\ f_B(E_2)$$
$$f_2(z_2 = +\infty) = f_1^{(0)}(E_1', r_1'; t)\ f_B(E_2')$$

where (E_1', r_1', E_2', r_2') evolves into (E_1, r_1, E_2, r_2) over the course of a collision.

Subsequently applying conservation of energy

$$E_1' + E_2' = E_1 + E_2$$

and detailed balance

$$\left[2\pi n\, r_1 \frac{\tau_z(E_1, r_1)}{m_e} f_B(E_1) \right] k(E_1, r_1 | \overline{E_1}, \overline{r_1}) =$$

$$\left[2\pi n\, \overline{r_1} \frac{\tau_z(\overline{E_1}, \overline{r_1})}{m_e} f_B(\overline{E_1}) \right] k(\overline{E_1}, \overline{r_1} | E_1, r_1)$$

where

$$\tau_z(E_1, r_1) = \oint_{E_1} \frac{dz_1}{v_1}$$

and

$$k(E_1, r_1 | \overline{E_1}, \overline{r_1}) = \frac{n}{\tau_z(E_1, r_1)} \oint_{E_1} \frac{dz_1}{v_1} \int d\vec{x}_{2\perp} dv_2 |v_2| f(E_2) \delta(\overline{E_1} - E_1') \delta(\overline{r_1} - r_1')$$

yields the **Master Equation**

$$\frac{\partial \rho(E_1, r_1; t)}{\partial t} = \int d\overline{E_1} d\overline{r_1} \left[\rho(\overline{E_1}, \overline{r_1}; t) k(\overline{E_1}, \overline{r_1} | E_1, r_1) - \rho(E_1, r_1; t) k(E_1, r_1 | \overline{E_1}, \overline{r_1}) \right]$$

where

$$\rho(E_1, r_1; t) = 2\pi r_1 W(E_1, r_1; t) .$$