Microscopic Diffusion in Stellar Plasmas

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OUTLINE

What is a plasma and miscellaneous considerations
  Debye shielding

Description of stellar plasmas
  Chapman-Enskog theory
    Approximate solutions

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  Burgers equations
    Approximate solutions

Collision integrals

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Summary

What is a plasma?

a gas made of charged particles which
behave in a « collective » manner

Kinetic energy of the particles must be much larger
than the electrostatic potential energy

\[ e\phi \ll kT \]
Debye shielding

Poisson equation: \[ \nabla^2 \phi = -4\pi \rho = 4\pi e(n_e - n_i) \]

at equilibrium (H⁺-e⁻ plasma)

\[ n_e = n_0 e^{\phi / kT} \sim n_0 (1 + e^{\phi / kT}) \]
\[ n_i = n_0 e^{-\phi / kT} \sim n_0 (1 - e^{\phi / kT}) \]

\[ \Rightarrow \left\{ \begin{array}{l}
\nabla^2 \phi = 4\pi e n_0 \frac{2e\phi}{kT} = \lambda_D^{-2} \phi \\
\lambda_D = \sqrt{\frac{kT}{8\pi e^2 n_0}}
\end{array} \right. \]

\[ \Rightarrow \phi = (q/R)e^{-r/\lambda_D} \]

i.e.: not a « pure » Coulomb potential, but a « shielded » potential

assumption: \( e\phi \ll kT \)

\[ \Rightarrow \frac{e\phi}{kT} \sim \frac{eq/r}{kT} \sim \frac{e^2}{kT a_0} \sim \frac{e^2}{kT n_0^{-1/3}} \ll 1 \]

\[ \Rightarrow n_0 \left( \frac{kT}{e^2} \right)^{3/2} \sim n_0 \lambda_D^3 \gg 1 \]

i.e. many particles in a Debye sphere
Concept of « shielding » only valid if there are many particles in a Debye sphere, i.e. if $\Lambda = n_0 \lambda_D^3 \gg 1$.

NOTE: In astro papers, the plasma parameter $\Lambda$ is defined differently, as $\Lambda = 1/(4\pi n_0 \lambda_D)$, i.e., the inverse of the $\Lambda$ defined here. Therefore, in astro papers, $\Lambda \ll 1$ will be used to characterize a weakly coupled plasma!

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Equations for stellar plasmas

The diffusion equation is obtained by solving (with some approximations) the Boltzmann equation for binary or multiple gas mixtures.

\[ \frac{\partial f_i}{\partial t} + \vec{v}_i \cdot \frac{\partial f_i}{\partial \vec{r}} + F_i \frac{\partial f_i}{\partial \vec{v}_i} = \partial \gamma \frac{\partial f_i}{\partial t} \]

Two methods have been used:

• Chapman-Enskog theory

• Burgers’ equations

In both methods, the diffusion coeff. can be written as functions of the collision integrals, which depend on the exact nature of the interaction between colliding particles.

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Chapman-Enskog theory

The total distribution function of a given species can be written as a convergent series, each term representing a successive approximation to the distribution function:

\[ f_i(r', \dot{v}, t) = f_i^{(0)}(r', \dot{v}, t) + f_i^{(1)}(r', \dot{v}, t) + f_i^{(2)}(r', \dot{v}, t) + \ldots \]

\[ \frac{|f_i^{(n)}|}{|f_i^{(n-1)}|} \ll 1 \]

- Substitute into Boltzmann equation
- Linearize
- Get series of equations for each \( f_i^{(n)} \) in terms of lower order approx.

\( f_i^{(0)} \) is a Maxwellian distribution function characterized by \( n_i, T, v_0 \)

These parameters and their derivatives enter into successive approx. of the total distribution function and define the transport properties.

Transport coefficients are obtained by taking velocity moments of the first-order approximation of the distribution function.

Good estimates of the diffusion coefficients are given by the so-called first and second approximations to transport properties (obtained by expanding the first-order distribution function on the basis of Sonine polynomials, which gives a very rapidly convergent series (Chapman & Cowling 70))
Binary mixture

Chapman & Cowling 70

\[ v_2 - v_1 = -D_{12} \left\{ \frac{n^2}{n_1 n_2} \nabla \left( \frac{n_2}{n_1} \right) + \frac{m_1 - m_2}{\mu} \nabla \ln p + \frac{n^2}{n_1 n_2 D_{12}} D_{th} \nabla \ln T - \frac{m_1 m_2}{\mu k T} (F_2 - F_1) \right\} \]

- thermal diffusion coeff.
- molecular diffusion coeff.
- reduced mass
- external forces (e.g., electric or radiation force)

Atom-test approximation

\[ v_2 - v_1 = -D_{12} \left\{ \frac{n^2}{n_1 n_2} \nabla \left( \frac{n_2}{n_1} \right) + \frac{m_1 - m_2}{\mu} \nabla \ln p + \frac{n^2}{n_1 n_2 D_{12}} D_{th} \nabla \ln T - \frac{m_1 m_2}{\mu k T} (F_2 - F_1) \right\} \]

Assume \( n_2 << n_1 \)

\[ \Rightarrow v_2 = D_{12} \left\{ \nabla \ln c \mid \left( \frac{m_2}{m_1} \right) \nabla \ln p \mid \alpha_T \nabla \ln T \frac{m_2 (F_2 - F_1)}{k T} \right\} \]

- \( c = n_2 / n \)
- \( \alpha_T = \left( 1 / c \right) \left( D_{th} / D_{12} \right) \)
Element diffusion driven by $\nabla p$ (or $\nabla g$), $\nabla T$, $\nabla C_i$

Electrons tend to rise but held back by $E$ which counteracts $g$

Heavier elements tend to sink towards the center

$\nabla T \Rightarrow$ thermal diffusion $\Rightarrow$ tends to concentrate more highly charged and more massive particles towards hottest regions, i.e. center

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Burgers’ equations

Based on the Grad13 moment approximation and the use of a Fokker-Planck collision term in the Boltzmann equation.

i.e. computation of higher order moments of the Boltzmann equation, which allows a more direct evaluation of physical quantities of interest.

The main advantage over the Chapman & Cowling method is that it provides a more convenient way for handling multicomponent gases.

In the limit where collisions are very frequent and the temperatures of the various species are the same (collision-dominated plasma) the two methods are equivalent.

Underlying assumptions in Burgers equations:

1. Neglect radiative forces
2. Complete ionization
3. Maxwellian velocity distributions and same T for all species
4. Diffusion velocities << thermal velocities
5. No magnetic field
6. Collisions dominated by classical interactions between particles
7. Plasma is a dilute gas, i.e., ideal gas equation of state applies

6 and 7 not true when \( \Lambda = n_0 \lambda_B^3 \) is not >> 1

In this case transport properties from Boltzmann equation wrong Quantum effects and dynamical shielding should be taken into account
**Burgers’ equations**

- **mass conservation**
  \[
  \frac{\partial n_i}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 n_i w_i \right) = \left( \frac{\partial n_i}{\partial t} \right)_{\text{num}}
  \]

- **momentum conservation**
  \[
  \frac{\partial p_i}{\partial r} + \rho_i g - \rho_{ei} E = \sum_{j \neq i} K_{ij} (w_j - w_i) + \sum_{j \neq i} \frac{m_j r_i - m_i r_j}{m_i + m_j}
  \]

- **energy conservation**
  \[
  \frac{5}{2} n_i k_B \frac{dT}{dr} = -\frac{5}{2} \sum_{j \neq i} K_{ij} z_{ij} \frac{m_i}{m_i + m_j} (w_j - w_i) - \frac{2}{5} K_{ii} z_{ii} r_i
  \]
  \[
  + \sum_{j \neq i} \frac{K_{ij} m_i m_j}{(m_i + m_j)^2} \left( 3 - z_{ij}^' - 0.8z_{ij}^" \right) r_i
  \]

**Constraints**

- **Local mass conservation**
  \[
  \sum_{i} m_i n_i w_i = 0
  \]

- **Current neutrality**
  \[
  \sum_{i} q_i n_i w_i = 0
  \]

- **Charge neutrality**
  \[
  \sum_{i} q_i n_i = 0
  \]
Burgers equations + constraints

= closed system of LINEAR equations for:

- the diffusion velocities \( w_i \)
- the residual heat flow vectors \( r_i \)
- the gravitational acceleration \( g \)
- the electric field \( E \)

in terms of:

- the pressure \( p \)
- the temperature \( T \)
- the concentration gradients \( C_i = n_i/n_e \)

Main difficulty: Collision integrals (resistance coefficients)

Otherwise, the linear system can be solved analytically, but it is long and tedious!

2 solutions:

- simplify (additional approximations)
- resolve numerically
Simplified solutions

Ignore the residual heat fluxes: $r_s = 0$

→ no need for the energy equation

\[
\frac{\partial \rho_i}{\partial r} + \rho_i g - \rho_c i E = \sum_{j \neq i} K_{ij} (w_j - w_i)
\]

Much easier to solve!

For a pure Hydrogen-Helium-electrons plasma:

\[
w_H = \frac{kT n_H}{K_{HHc}} \frac{1 - X}{2X} \left[ \frac{5}{4} (1 - X) \frac{d \ln p}{dr} + \frac{(X + 3)}{(X - 1)(5X - 3)} \frac{d \ln X}{dr} \right]
\]

the collisions with the electrons have been neglected and $m_e/m_i \ll 1$

Michaud & Proffitt 1993: for trace H, underestimation by 30%

For a trace element in a H-He background:

see formula by Michaud & Proffitt 93

OK for pure H or pure He, otherwise large errors
They add an empirically determined thermal diffusion velocity
Numerical solution

Fortran routine from Thoul, Bahcall & Loeb 94
is freely available

Note: as mentioned in the accompanying README file, there is a typo in equation 9 of TBL94, which should read

\[
\ln \Lambda_{st} = \frac{1.6249}{2} \ln \left[ 1 + 0.18769 \left( \frac{4k_B T \lambda}{Z_s Z_t e^2} \right)^{1.2} \right]
\]
The resistance coefficients

\[ K_{ij} \quad \pi_{ij} \quad \pi_{ij}' \quad \pi_{ij}'' \]

1. Pure Coulomb potential: diverges

2. Pure Coulomb potential with cutoff at the Debye length: easy (analytic)

\[ V_{ij} = \frac{Z_i Z_j e^2}{r} e^{-r/\lambda_D} \]

3. Shielded Debye-Hückel potential: better

4. Modified Debye-Hückel potential: even better

\[ V_{ij} = \frac{Z_i Z_j e^2}{r} e^{-r/\text{max}(\lambda_D, a_0)} \]

5. With quantum corrections: best

---

truncated Coulomb potential: \( \pi_{ij} = 0.6, \quad \pi_{ij}' = 1.3, \quad \pi_{ij}'' = 2 \)

- momentum conservation

\[
\frac{\partial p_i}{\partial r} + \rho_i g - \rho_e \varepsilon = \sum_{j \neq i} K_{ij} [(w_j - w_i) + 0.6(x_{ij} r_i - y_{ij} r_j)]
\]

- energy conservation

\[
\frac{5}{2} n_e k_B \frac{dT}{dr} = \sum_{j \neq i} K_{ij} \left\{ \frac{3}{2} x_{ij} (w_i - w_j) - y_{ij} [1.6 x_{ij} (r_i + r_j) + Y_{ij} r_i - 4.3 x_{ij} r_j] \right\}
\]

\[ \rightarrow \text{Solved numerically (i.e. no approximation)} \]
\[ \text{in TBL94's routine} \]
Coulomb Logarithm

\[ K_{ij} = \frac{2^{3/2}}{3} e^{\frac{1}{4}} Z_i^2 Z_j^2 n_i n_j \left( \frac{m_i m_j}{m_i + m_j} \right)^{1/2} (k_B T)^{-3/2} 2 \ln \Lambda_{ij} \]

Coulomb logarithm: many different approximations/fits

- Modified Debye-Hückel potential at low densities and Thomas-Fermi potential at high densities
- Calculated by Fontaine & Michaud (79)
- Fitted by Iben & MacDonald (85)

\[ 2 \ln \Lambda_{ij} = 1.6249 \ln (1 + 0.18769 \frac{4 k_B T \lambda}{Z_i Z_j e^2})^{1.2} \]

\[ \lambda = \max (\lambda_D, a_0) \]

\[ \lambda_D = \left( \frac{k_B T}{4 \pi e^2 \sum n_s Z_s^2} \right)^{(1/2)} \]

\[ a_0 = \left( \frac{3}{4 \pi \sum_{\text{ions}} n_i} \right)^{1/3} \]

Debye length

interionic distance

(Used in Thoul & al 94 diffusion routine)
• Michaud & Proffitt 93: replace the Coulomb logarithm by $C_{ij}$ which is a function of \( \frac{2kT\lambda}{Z_i Z_j e^2} \)

\[
\ln \Lambda_{ij} = 2^{3/2} \sqrt{\pi} \varepsilon^4 r^2 \frac{1}{n_i n_j} \left( \frac{m_i m_j}{m_j} \right)^{1/2} (kT)^{-3/2} \epsilon \nabla
\]

NOTE:
Here, $\ln \Lambda_{ij}$ is as in MP93 (and others). IT IS DIFFERENT FROM $\ln \Lambda_{ij}$ in TBL94 (and others).

\( (2 \ln \Lambda_{ij})_{TBL} = (\ln \Lambda_{ij})_{MP} \)

If the heavy elements can be ignored in $\lambda_0$ then

\[
\ln \Lambda_{XY} = -19.95 - \frac{1}{2} \ln \rho + \frac{3}{2} \ln T - \frac{1}{2} \ln \frac{X+3}{2}
\]

Comparisons

• Truncated Coulomb potential: $z_{ij} = 0.6$, $z'_{ij} = 1.3$, $z''_{ij} = 2$

• Modified Debye-Hückel potential: Paquette & al 86’s fitted by Michaud & Proffitt 93

Truncated pure Coulomb potential is OK in the low density limit
More accurate calculations at high densities
MacDonald 91

Iben & MacDonald 85

fit to Fontaine & Michaud 79

dense plasma
dilute plasma
Using $\ln \Lambda_{ij}$ as an approx. for $C_{ij}$ is OK in the low density limit.
Comparison between fit by Iben & MacDonald 85 and Paquette et al’s 86 (Iben,Fujimoto & MacDonald 92)

![Graph showing comparison between different fits for high and low densities.]

Schlattl & Salaris 2003

Compare several classical calculations
⇒ all very close

Main sequence stars: $\phi$ remains very close to 2 for H and He ⇒ constant values can be assumed
Quantum corrections increase the efficiency of diffusion. Their effect is more pronounced at higher densities.

Note that the uncertainty on the diffusion coefficients is still ~10% due to the use of Burgers’ formalism, which is only equivalent to the Chapman & Cowling’s second-order approximation.
Sound speed in the Sun
(Basu97-solar model)/Basu97

SS03 = most accurate resistance coeff. currently available
By chance, Thoul et al 94 gives the closest results for the Sun

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Descriptions of stellar plasmas: all based on Boltzmann equation
In interior of main-sequence stars, $\Lambda \sim 1$, i.e. not a "classical" plasma.
⇒ careful with validity of Boltzmann equation
⇒ No physically correct theory

Two theories: - Chapman-Enskog     - Burgers
Chapman-Cowling = for a H+e+trace ion plasma
Burgers equivalent to 2nd-order Chapman-Cowling (ok in weakly coupled plasmas)
More accurate results would be obtained with a higher-order approx. but untractable for a multicomponent gas
Burgers much more tractable for multicomponent gas

The problem of the collision integrals:
- easy in weakly coupled plasmas (pure Coulomb + cutoff at $\lambda_D$: analytic)
- shielded potential better but also only valid in weakly-coupled plasmas
- extrapolate to a modified Debye-Hückel ⇒ seems to give good results, but no physical argument
- recent quantum calculations available

Careful with the assumptions in the numerous approximations and fits
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