

Basic Physics Behind Operation of TPC

Part I

-- Fundamental Processes in the TPC --

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Purpose

Being a non-expert, I will focus on very basic principles, trying to introduce you, students excluding experts, to more advanced topics containing more practical and technical aspects to be covered by real experts in this school.

Emphasis will be put on concepts and philosophy, and hence practical examples will be minimum, for them take a look at excellent text books such as

V.Palldino & B.Sadoulet 1974: LBL-3013

F.Sauli 1977: CERN 77-09

W.Blum & L.Rolandi 1993

Fundamental Processes

Beam



Ionizations

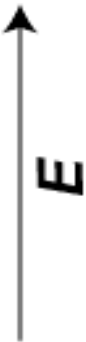
→ Liberation of Electrons

$$P_I(N; \bar{N})$$

Normal incidence
(no angle effect)

No δ -ray

Drift Volume



Drift electrons

Drift and Diffusion

$$P_D(x_i; \sigma_d) = \frac{1}{\sqrt{2\pi}\sigma_d} \exp\left(-\frac{x_i^2}{2\sigma_d^2}\right)$$

$$\sigma_d = C_d\sqrt{z}$$

Amplification Gap

Amplification and further Diffusion

$$P_G(G/\bar{G}; \theta) = \frac{(\theta + 1)^{\theta+1}}{\Gamma(\theta + 1)} \left(\frac{G}{\bar{G}}\right)^\theta \exp\left(-(\theta + 1) \left(\frac{G}{\bar{G}}\right)\right)$$

Readout Pads



Pad Response

Coordinate

x



Subjects to be Covered

- ▲ Liberation of electrons by ionization (dE/dx)
- Classical theory of electron transportation in a chamber gas and its applications
 - Behaviors of electrons in E and B fields
 - Transport coefficients: V_d , C_d
 - Gas amplification
 - Creation of signals
- Coordinate measurement

Subjects Left Out

- Electron attachment
 - CF₄, O₂ contamination, etc.
- Transportation of ions
 - +ve ion feed back
 - Ion exchange and aging

These are very important in practice, but simply beyond the scope of my lectures.

Classical Theory of Electrons in a Gas

Boltzmann Equation

Basic Equation Governing Electron Transportation

- We often see formulae for electron drift and diffusion as derived from it, so it must be useful, but itself is rarely discussed in an usual introductory text books.
- So, what is it?
- Where does it come from?
- And how?

- I can only show you a rough sketch, but I hope it will make you feel a little bit more comfortable when you see it next time.
- For (older) pragmatic people, it might become a little bit boring, but maybe it's OK even for them to recall their student time.

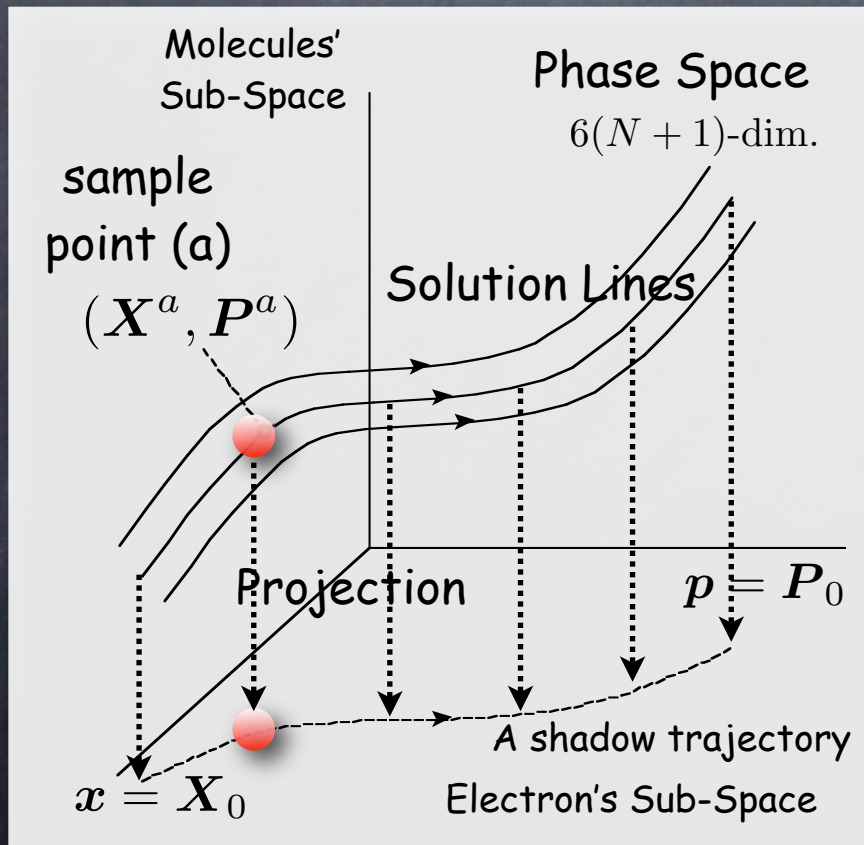
We will find that **THE KEY WORD IS "PROJECTION"!**

"PROJECTION" is a technique to forget about unwanted details and make life easy!

Phase Space

Stage where solutions dance, we only see their shadows

- Our system of interest
 - Ionization electrons drift and diffuse independently
 - It suffices to consider a single electron in a gas consisting of N gas molecules in a chamber (note: N is a huge number).



Microscopic Picture

Causal deterministic motion by

$$H = \frac{p^2}{2m} + \sum_{b=1}^N \frac{P_b^2}{2M_b} + U_{\text{ext}}(\mathbf{x}, \mathbf{p}) + U_{\text{mM}}(\mathbf{x}, \mathbf{X}) + U_{\text{MM}}(\mathbf{X}, \mathbf{X}')$$

: Lorentz force (E,B)
: elec. + mol. collision
: mol. + mol. collision

Macroscopic Picture

Projection = Coarsification
= information loss

Stochastic probabilistic motion

Liouville's Theorem

Solutions flow as perfect incompressible fluid

Hamiltonian Equation of Motion

Motion of a phase space point:

$$\Phi = \begin{pmatrix} X \\ P \end{pmatrix}$$

satisfies

$$\dot{\Phi} = \frac{\partial H}{\partial \bar{\Phi}^T} \quad \text{with} \quad \bar{\Phi} = \begin{pmatrix} P \\ -X \end{pmatrix}$$

Time Evolution Operator

Write its formal solution as

$$\Phi(t) = D(t) \Phi(0)$$

then this is a 1-to-1 map because of the uniqueness of solution

$D(t)$ forms an Abelian group

$$D(t_1)D(t_2) = D(t_1 + t_2)$$

$$D(0) = 1$$

$$D(-t)D(t) = D(t - t) = D(0) = 1$$

Liouville's Theorem

$$J(t) = \det \left(\frac{\partial D(t) \Phi}{\partial \Phi} \right) = 1$$

The map preserves phase space volume

Liouville's Equation

$$\rho(\Phi; t) = \rho(X, P; t) \quad \begin{array}{l} \text{State density} \\ \text{function} \end{array}$$

$$0 = \frac{\partial}{\partial t} \rho + \frac{\partial H}{\partial \bar{\Phi}} \frac{\partial}{\partial \Phi^T} \rho$$

Proof of Liouville's Eq.

Proof is easy enough to give here

Proof of Liouville's Theorem

Equation of motion says

$$D(dt)\Phi = \Phi + dt \dot{\Phi} = \Phi + dt \frac{\partial H}{\partial \bar{\Phi}^T}$$

resulting in

$$\frac{\partial D(dt)\Phi}{\partial \Phi} = 1 + dt \frac{\partial^2 H}{\partial \bar{\Phi}^T \partial \Phi}$$

We hence have

$$\begin{aligned} \det \left(\frac{\partial D(dt)\Phi}{\partial \Phi} \right) &= 1 + dt \operatorname{Tr} \left(\frac{\partial^2 H}{\partial \bar{\Phi}^T \partial \Phi} \right) + O((dt)^2) \\ &= 1 + O((dt)^2) \end{aligned}$$

$$\frac{1}{dt} (J(dt) - 1) = \frac{1}{dt} (J(dt) - J(0)) = \frac{d}{dt} J(0) = 0$$

which leads us to

$$\begin{aligned} \frac{d}{dt} J(t) &= \lim_{t_1 \rightarrow t} \frac{\partial}{\partial t} \det \left[\left(\frac{\partial D(t-t_1)D(t_1)\Phi}{\partial D(t_1)\Phi} \right) \left(\frac{\partial D(t_1)\Phi}{\partial \Phi} \right) \right] \\ &= \lim_{t_1 \rightarrow t} \frac{\partial}{\partial t} \left[\det \left(\frac{\partial D(t-t_1)D(t_1)\Phi}{\partial D(t_1)\Phi} \right) \right] \cdot \left[\det \left(\frac{\partial D(t_1)\Phi}{\partial \Phi} \right) \right] \\ &= \left[\frac{d}{dt} J(0) \right] \cdot J(t_1) = 0 \quad \therefore J(t) = 1 \end{aligned}$$

Derivation of Liouville's Equation

In general, for any observable A :

$$\begin{aligned} \frac{d}{dt} A(\Phi; t) &= \dot{\Phi} \frac{\partial}{\partial \Phi^T} A(\Phi; t) + \frac{\partial}{\partial t} A(\Phi; t) \\ &= \frac{\partial H}{\partial \bar{\Phi}} \frac{\partial}{\partial \Phi^T} A(\Phi; t) + \frac{\partial}{\partial t} A(\Phi; t) \end{aligned}$$

Since Liouville's theorem requires that the state density stays unchanged, which implies

$$0 = \frac{d}{dt} \rho = \frac{\partial H}{\partial \bar{\Phi}} \frac{\partial}{\partial \Phi^T} \rho + \frac{\partial}{\partial t} \rho$$

This is actually a continuity equation in the full phase space of the system or conservation of probability:

$$\int d^{6(N+1)} \Phi \rho(\Phi; t) = 1$$

State Density Function

All we know about the ensemble

Microscopic Picture

Once an initial distribution is given, the state density function evolves deterministically according to Liouville's equation.

$$\rho(\Phi; t) = \rho(D(-t)\Phi; 0)$$

But how should we fix the initial distribution?

Ergodic hypothesis:

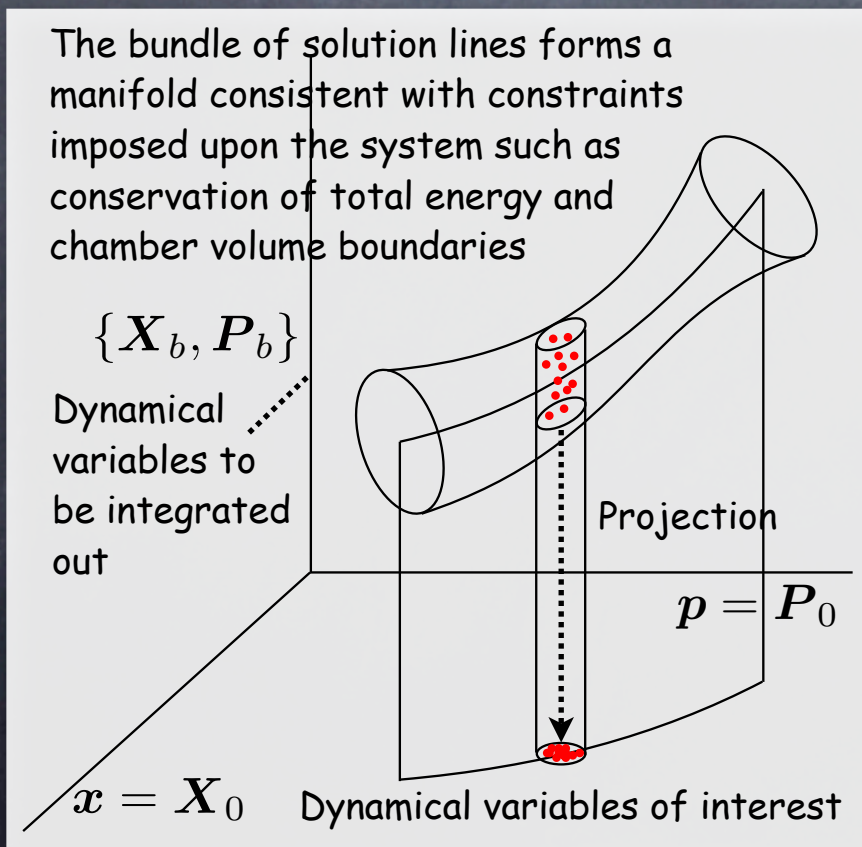
Probability is proportional to phase space volume

Thermal equilibrium = Equal weight

Macroscopic Picture

Projection = Coarsification
= information loss

Projected volume decides probability



Maxwellian Distribution

A detour which proves the power of ergodic hypothesis

State Density Function for Molecules

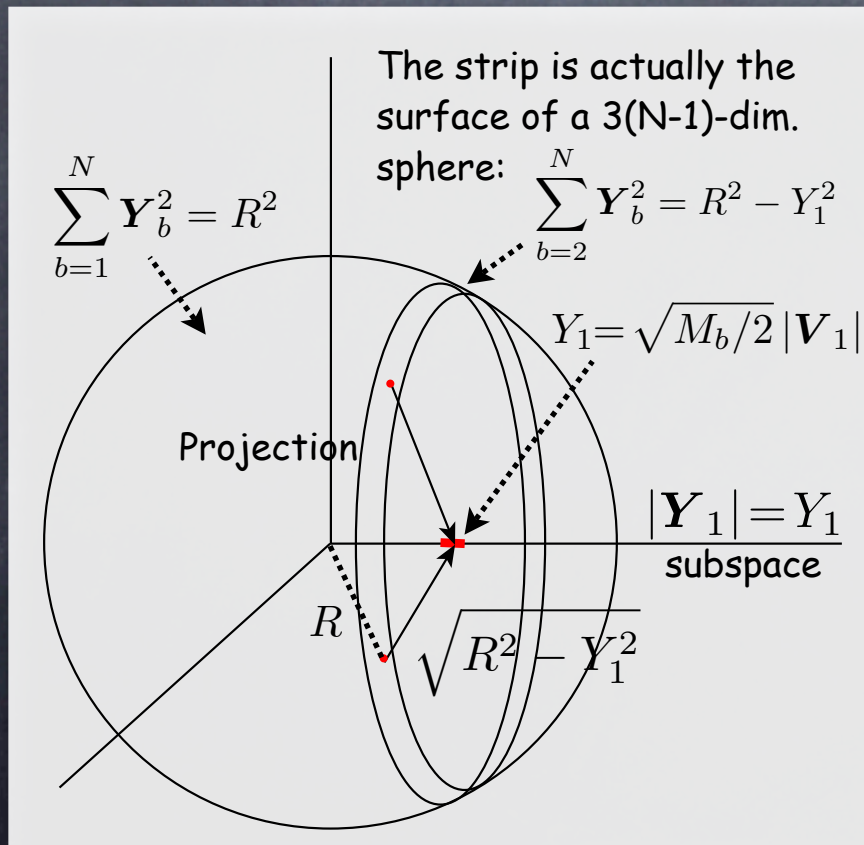
Ignore the electron, for the moment, and concentrate on the molecules, whose state density function in thermal equilibrium. Good approximation since we can safely assume that the molecules colliding with the electron never met it in the past.

Interaction hamiltonian of the molecules has a nonzero value only when the inter-molecule distance becomes negligibly small compared to its average determined by the gas density.

$$E_{\text{tot}} = \sum_{b=1}^N \frac{1}{2} M_b V_b^2 := \sum_{b=1}^N Y_b^2 = R^2$$

The phase space points uniformly distribute over the surface of a $3N$ -dim. sphere of radius $R = \sqrt{E_{\text{tot}}}$ \times $3N$ -dim. box with a volume L^{3N} . Note that the projection of spatial dimension simply gives L^{3N} .

$$\begin{aligned} & S_{3(N-1)} \left(\sqrt{R^2 - Y_1^2} \right) \\ & \propto \left(\sqrt{R^2 - Y_1^2} \right)^{3(N-1)-1} \approx R^{3N-4} \left[1 - (Y_1/R)^2 \right]^{3N/2} \\ & \approx R^{3N-4} \left[1 - \frac{Y_1^2 / ((2/3)R^2/N)}{3N/2} \right]^{3N/2} \\ & \rightarrow R^{3N-4} \exp \left[-\frac{Y_1^2}{(2/3)(R^2/N)} \right] \propto \exp \left[-\frac{Y_1^2}{k_B T} \right] \end{aligned}$$



Projection of Liouville's Eq.

Electron distribution as the projection of the full state fun.

Liouville's Equation

$$\rho(\Phi; t) = \rho(\mathbf{X}, \mathbf{P}; t) \quad \text{State density function}$$
$$0 = \frac{\partial}{\partial t} \rho + \frac{\partial H}{\partial \Phi} \frac{\partial}{\partial \Phi^T} \rho$$

Separating the part containing the electron's dynamical variables from the rest, we have

$$0 = \left[\frac{\partial}{\partial t} + \frac{\mathbf{p}}{m} \cdot \frac{\partial}{\partial \mathbf{x}} + \mathbf{F}_{\text{ext}} \cdot \frac{\partial}{\partial \mathbf{p}} \right] \rho$$
$$+ \sum_{b=1}^N \mathbf{F}_b \cdot \left[\frac{\partial}{\partial \mathbf{p}} - \frac{\partial}{\partial \mathbf{P}_b} \right] \rho_b$$

+ Molecule Only Terms

Now project the both sides to the electron subspace by integrating out molecules' dynamical variables

Notice that

$$\mathbf{F}_{\text{ext}} = e \left[\mathbf{E} + \frac{\mathbf{p}}{mc} \times \mathbf{B} \right] \quad (e < 0)$$

The "molecule only" terms become surface integrals upon integration and vanish because rho has the same value everywhere on the surface.

$$0 = \left[\frac{\partial}{\partial t} + \frac{\mathbf{p}}{m} \cdot \frac{\partial}{\partial \mathbf{x}} + \mathbf{F}_{\text{ext}} \cdot \frac{\partial}{\partial \mathbf{p}} \right] f$$
$$+ \sum_{b=1}^N \int d^3 \mathbf{X}_b \int d^3 \mathbf{P}_b \mathbf{F}_b \cdot \left[\frac{\partial}{\partial \mathbf{p}} - \frac{\partial}{\partial \mathbf{P}_b} \right] f_b$$

where we have introduced

1-body distribution function:

$$f(\mathbf{x}, \mathbf{p}; t) = \prod_{b'=1}^N \left(\int d^6 \Phi_{b'} \right) \rho(\mathbf{x}, \mathbf{p}; \{\Phi_{b'}\}; t)$$

2-body distribution function:

$$f_b(\mathbf{x}, \mathbf{p}; \mathbf{X}_b, \mathbf{P}_b; t) = \prod_{b' \neq b} \left(\int d^6 \Phi_{b'} \right) \rho(\mathbf{x}, \mathbf{p}; \Phi_b, \{\Phi_{b'}\}; t)$$

Collision Term

Time average over the collision period

Collision Term

We move the 2-body term to the R.H.S. and call it the collision term:

$$\left(\frac{\partial f}{\partial t}\right)_{\text{coll}} = - \sum_{b=1}^N \int d^3 X_b \int d^3 P_b F_b \cdot \left[\frac{\partial}{\partial \mathbf{p}} - \frac{\partial}{\partial \mathbf{P}_b} \right] f_b$$

for obvious reason. Notice that if it were not for this term, the electron would have behaved as a single particle in external E and B fields.

With this term, however, the projected trajectory of the electron will show a shaggy apparently random motion, though the full trajectory should be smooth and causal in the full phase space.

Noting that the 2-body system can be regarded as isolated during the short period of collision time and the collision motion averaged using the projected H:

$$\begin{aligned} \bar{H}_2(\mathbf{x}, \mathbf{p}; \mathbf{X}_b, \mathbf{P}_b) &= \frac{\prod_{b' \neq b} \left(\int d^3 X_{b'} \int d^3 P_{b'} \right) H(\Phi)}{\prod_{b' \neq b} \left(\int d^3 X_{b'} \int d^3 P_{b'} \right)} \\ &= \frac{\mathbf{p}^2}{2m} + \frac{\mathbf{P}_b^2}{2M_b} + U_{\text{mM}}(|\mathbf{x} - \mathbf{X}_b|) \end{aligned}$$

which is none other than the 2-body Hamiltonian describing the collision.

Then we have

$$\begin{aligned} - \int_{t-\frac{\Delta t}{2}}^{t+\frac{\Delta t}{2}} dt' F_b \cdot \left[\frac{\partial}{\partial \mathbf{p}} - \frac{\partial}{\partial \mathbf{P}_b} \right] f_b &= \int_{t-\frac{\Delta t}{2}}^{t+\frac{\Delta t}{2}} dt' \left(\frac{\partial f_b}{\partial t'} \right) \\ &= f_b \left(\phi_2; t + \frac{\Delta t}{2} \right) - f_b \left(\phi_2; t - \frac{\Delta t}{2} \right) \\ &= f_b \left(D_2(-\Delta t) \phi_2; t - \frac{\Delta t}{2} \right) - f_b \left(\phi_2; t - \frac{\Delta t}{2} \right) \end{aligned}$$

where $D_2(t')$ is the 2-body time evolution operator and

$$\phi_2 = (\mathbf{x}, \mathbf{p}; \mathbf{X}_b, \mathbf{P}_b)$$

is the 2-body phase space point in question.

Collision Term (Continued)

Decomposition of 2-body fn. to products of 1-body fns.

Before and after the collision period of the 2-body system, their space coordinates don't change macroscopically, but their momenta may seem to jump by a finite amount.

Microscopically, however, the jump is a function of the impact parameter and their relative momentum and should be causal in our classical mechanical treatment.

$$- \int_{t-\frac{\Delta t}{2}}^{t+\frac{\Delta t}{2}} dt' \mathbf{F}_b \cdot \left[\frac{\partial}{\partial \mathbf{p}} - \frac{\partial}{\partial \mathbf{P}_b} \right] f_b \\ = f_b \left(D_2(-\Delta t) \phi_2; t - \frac{\Delta t}{2} \right) - f_b \left(\phi_2; t - \frac{\Delta t}{2} \right)$$

Probabilistic view point enters upon replacing the 2-body state density function by the product of the 1-body state density functions for the electron and the molecule in question.

$$f_b(\phi_2; t) = f_b(\mathbf{x}, \mathbf{p}; \mathbf{X}_b, \mathbf{P}_b; t) \\ \approx f(\mathbf{x}, \mathbf{p}; t) F_b(\mathbf{P}_b; t)$$

Notice that the momentum transfer is determined by the relative momentum and the impact parameter. This replacement drops the information on the impact parameter by throwing away the coordinate information of the molecule. This loss of information is the source of the stochastic nature of the collision process.

We hence make the replacement

$$\int d^3 \mathbf{X}_b \rightarrow \int d\sigma_b |\mathbf{v} - \mathbf{V}_b| \Delta t \begin{pmatrix} \mathbf{p} & = & m\mathbf{v} \\ \mathbf{P}_b & = & M_b \mathbf{V}_b \end{pmatrix}$$

since the volume integral should be taken over the region where

$$D_2(-\Delta t) \neq 1$$

or over the X-section along the expected trajectory of the 2-body system.

Collision Term (Continued)

Time average over the collision period

Time Averaged Collision Term

Averaged over the collision time, we get

$$\begin{aligned} & \frac{1}{\Delta t} \int_{t-\frac{\Delta t}{2}}^{t+\frac{\Delta t}{2}} dt' \left(\frac{\partial f}{\partial t} \right)_{\text{coll}} \\ &= \sum_{b=1}^N \int d^3 \mathbf{P}_b \int d\sigma_b |\mathbf{v} - \mathbf{V}_b| \\ & \quad \times [f(\mathbf{x}, \mathbf{p} + \Delta \mathbf{q}; t) F_b(\mathbf{P}_b - \Delta \mathbf{q}; t) \\ & \quad - f(\mathbf{x}, \mathbf{p}; t) F_b(\mathbf{P}_b; t)] \end{aligned}$$

In what follows we understand the time derivative as appropriately averaged over the collision period as above, and simply write

$$\begin{aligned} \left(\frac{\partial f}{\partial t} \right)_{\text{coll}} &= \sum_{b=1}^N \int d^3 \mathbf{P}_b \int d\sigma_b |\mathbf{v} - \mathbf{V}_b| \\ & \quad \times [f(\mathbf{x}, \mathbf{p} + \Delta \mathbf{q}; t) F_b(\mathbf{P}_b - \Delta \mathbf{q}; t) \\ & \quad - f(\mathbf{x}, \mathbf{p}; t) F_b(\mathbf{P}_b; t)] \end{aligned}$$

Since the same kind of molecules should contribute equally to the summation (rho should be symmetric under exchange of the same kind of molecules), we can rewrite this to

$$\begin{aligned} \left(\frac{\partial f}{\partial t} \right)_{\text{coll}} &= \sum_k N_k \int d^3 \mathbf{P} \int d\sigma_k |\mathbf{v} - \mathbf{V}| \\ & \quad \times [f(\mathbf{x}, \mathbf{p} + \Delta \mathbf{q}; t) F_k(\mathbf{P} - \Delta \mathbf{q}; t) \\ & \quad - f(\mathbf{x}, \mathbf{p}; t) F_k(\mathbf{P}; t)] \end{aligned}$$

where N_k is the number of molecules of k-th kind. Noting

$$1 = \int d^3 \mathbf{X} \int d^3 \mathbf{P} F_k(\mathbf{P}; t) = L^3 \int d^3 \mathbf{P} F_k(\mathbf{P}; t)$$

we define the density of molecules of k-th kind $n_k = N_k/L^3$ and

$$\bar{F}_k(\mathbf{P}; t) = L^3 F_k(\mathbf{P}; t)$$

The Boltzmann Equation

The fundamental equation

Then we finally arrive at the Boltzmann equation:

$$\left[\frac{\partial}{\partial t} + \frac{\mathbf{p}}{m} \cdot \frac{\partial}{\partial \mathbf{x}} + \mathbf{F}_{\text{ext}} \cdot \frac{\partial}{\partial \mathbf{p}} \right] f(\mathbf{x}, \mathbf{p}; t)$$

$$= \sum_k n_k \int d^3 P \int d\sigma_k |\mathbf{v} - \mathbf{V}|$$

$$\times \left[\underbrace{f(\mathbf{x}, \mathbf{p} + \Delta \mathbf{q}; t)}_{\text{part flowing in}} \bar{F}_k(\mathbf{P} - \Delta \mathbf{q}; t) - \underbrace{f(\mathbf{x}, \mathbf{p}; t)}_{\text{part flowing out}} \bar{F}_k(\mathbf{P}; t) \right]$$

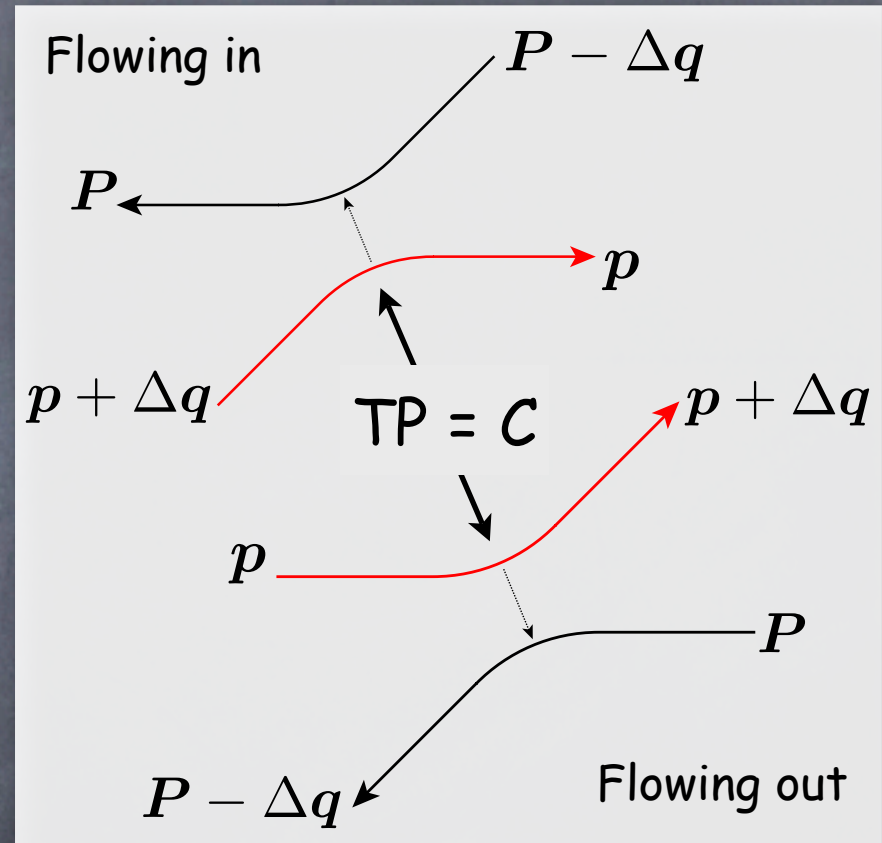
where the external force is given by

$$\mathbf{F}_{\text{ext}} = e \left[\mathbf{E} + \frac{\mathbf{v}}{c} \times \mathbf{B} \right]$$

and the velocities are defined by

$$\mathbf{p} = m\mathbf{v}$$

$$\mathbf{P} = M_k \mathbf{V}$$



Inelastic Scattering

A short comment in passing

So far, we have been assuming that the electron-molecule collisions are elastic as described by a scattering potential.

If we are to consider inelastic scattering involving some change of internal degrees of freedom of the colliding molecule, we need to expand the phase space to include the internal degrees of freedom and then project out these internal degrees of freedom as needed.

The resultant loss of information can again be taken statistically into account as the form of the inelastic cross section.

We can hence regard the Boltzmann eq. as the one after this extra projection.

The Boltzmann equation, as it is, can hence be applied to those more general cases.

In practice, however, the inclusion of inelastic processes complicate the treatment significantly, since we can no longer assume that the relative speed stays the same before and after the collision.

After all, the physics that controls the electron transport in a gas lies in the collision term, and that's where all the complications come from. Calculating the properties of complex molecules from the 1st principle (=Q.M.) is often impracticable.

Transport Coefficients

Things you want to derive from the Boltzmann Equation

- We often see formulae for electron drift and diffusion as derived from the Boltzmann equation, but they are given almost always without proof.
- Where do they come from?
- And how?
- I can only show you a rough sketch, but I hope it will make you feel a little bit more comfortable when you see them next time.
- Some of you, pragmatic people might already have been pretty much fed up, but be patient recalling your student time.

Again we will find THE KEY WORD IS "PROJECTION"!

"PROJECTION" makes life easy!

The Boltzmann Equation

From now on we will work in velocity space

The Boltzmann equation in (x, v) space is readily read out from its (x, p) version:

$$\left[\frac{\partial}{\partial t} + \mathbf{v} \cdot \frac{\partial}{\partial \mathbf{x}} + \frac{\mathbf{F}_{\text{ext}}}{m} \cdot \frac{\partial}{\partial \mathbf{v}} \right] f(\mathbf{x}, \mathbf{v}; t)$$

$$= \sum_k n_k \int d^3 \mathbf{V} \int d\sigma_k |\mathbf{v} - \mathbf{V}|$$

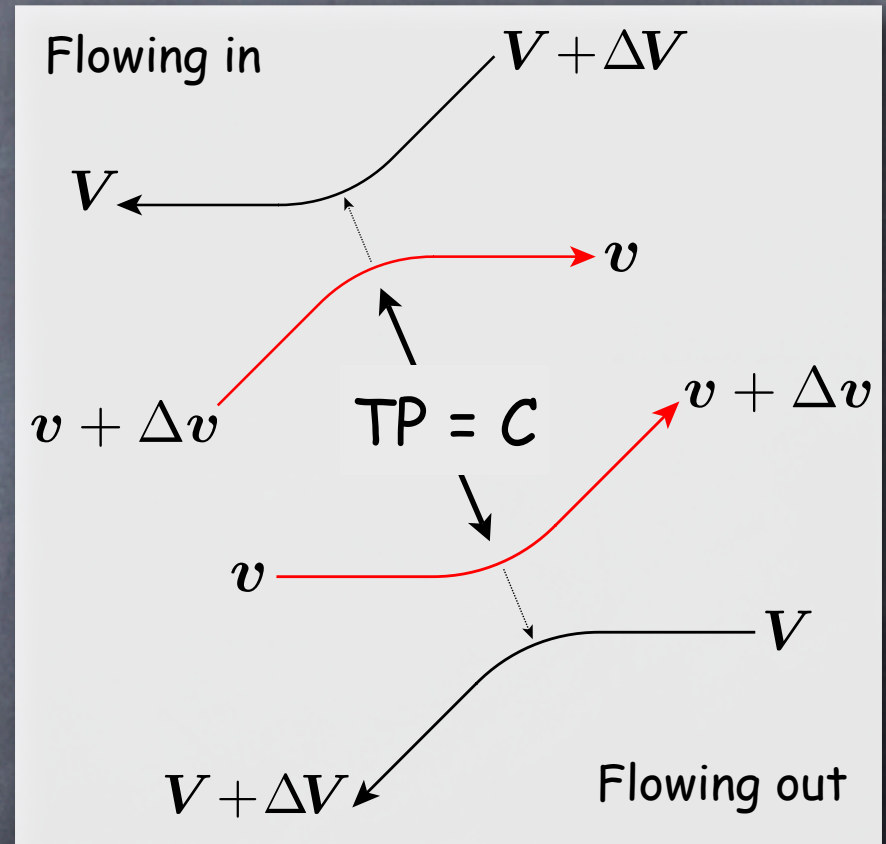
$$\times \left[\underbrace{f(\mathbf{x}, \mathbf{v} + \Delta \mathbf{v}; t) \bar{F}_k(\mathbf{V} + \Delta \mathbf{V}; t)}_{\text{part flowing in}} - \underbrace{f(\mathbf{x}, \mathbf{v}; t) \bar{F}_k(\mathbf{V}; t)}_{\text{part flowing out}} \right]$$

where the external force is given by

$$\mathbf{F}_{\text{ext}} = e \left[\mathbf{E} + \frac{\mathbf{v}}{c} \times \mathbf{B} \right]$$

and the velocity changes must satisfy

$$\Delta \mathbf{q} = m \Delta \mathbf{v} = -M_k \Delta \mathbf{V}$$



Before moving on, it is worth noting that the Boltzmann eq. implies a scale between the gas density and the field strengths for steady state solutions having no $(x; t)$ dependence.

Velocity Space

Decomposition of $f(\mathbf{x}, \mathbf{v}; t)$ to $n(\mathbf{x}; t) \bar{f}(\mathbf{v}; \mathbf{x}, t)$

The probability density of finding the electron in the vicinity of \mathbf{x} is given by

$$n(\mathbf{x}; t) = \int d^3 \mathbf{v} f(\mathbf{x}, \mathbf{v}; t)$$

With this, we can define the velocity distribution function by

$$\bar{f}(\mathbf{v}; \mathbf{x}, t) := f(\mathbf{x}, \mathbf{v}; t) / n(\mathbf{x}; t)$$

By definition this must satisfy the normalization condition:

$$\int d^3 \mathbf{v} \bar{f}(\mathbf{v}; \mathbf{x}, t) = 1$$

as is obvious by integrating both sides of the following over velocities

$$f(\mathbf{x}, \mathbf{v}; t) = n(\mathbf{x}; t) \bar{f}(\mathbf{v}; \mathbf{x}, t)$$

Putting this into the Boltzmann equation, we have

$$\begin{aligned} & \left[\frac{\partial}{\partial t} + \mathbf{v} \cdot \frac{\partial}{\partial \mathbf{x}} + \frac{\mathbf{F}_{\text{ext}}}{m} \cdot \frac{\partial}{\partial \mathbf{v}} \right] (n \bar{f}) \\ &= n(\mathbf{x}; t) \sum_k n_k \int d^3 \mathbf{V} \int d\sigma_k |\mathbf{v} - \mathbf{V}| \\ & \quad \times [\bar{f}(\mathbf{v} + \Delta \mathbf{v}; \mathbf{x}, t) \bar{F}_k(\mathbf{V} + \Delta \mathbf{V}; t) \\ & \quad - \bar{f}(\mathbf{v}; \mathbf{x}, t) \bar{F}_k(\mathbf{V}; t)] \end{aligned}$$

Notice that on the R.H.S. (collision term), $n(\mathbf{x}; t)$ has been factored out, since the collision is a very local phenomenon.

It is tempting to assume that \bar{f} will soon become independent of position and time due to random collisions with molecules, but this turns out incorrect as we will see next.

Simple Minded Factorization

$f(\mathbf{x}, \mathbf{v}; t) = n(\mathbf{x}; t) \bar{f}(\mathbf{v})$ does not work!

Integrating both sides of the B.Eq. over the electron velocities, we have

$$\begin{aligned} & \left[\frac{\partial}{\partial t} + \frac{\partial}{\partial \mathbf{x}} \cdot \langle \mathbf{v} \rangle + \int d^3 \mathbf{v} \frac{\mathbf{F}_{\text{ext}}}{m} \cdot \frac{\partial \bar{f}}{\partial \mathbf{v}} \right] n(\mathbf{x}; t) \\ &= n(\mathbf{x}; t) \int d^3 \mathbf{v} \sum_k n_k \int d^3 \mathbf{V} \int d\sigma_k |\mathbf{v} - \mathbf{V}| \\ & \quad \times [\bar{f}(\mathbf{v} + \Delta \mathbf{v}; \mathbf{x}, t) \bar{F}_k(\mathbf{V} + \Delta \mathbf{V}; t) \\ & \quad - \bar{f}(\mathbf{v}; \mathbf{x}, t) \bar{F}_k(\mathbf{V}; t)] \end{aligned}$$

where

$$\langle \mathbf{v} \rangle := \int d^3 \mathbf{v} \bar{f}(\mathbf{v}; \mathbf{x}, t) \mathbf{v}$$

is the local average velocity, which is in general position dependent.

If we assume a simple minded factorization

$$f(\mathbf{x}, \mathbf{v}; t) \approx n(\mathbf{x}; t) \bar{f}(\mathbf{v})$$

and integrate the both sides of the B.Eq. over the electron positions, noting

$$\int d^3 \mathbf{x} n(\mathbf{x}; t) = 1$$

we have

$$\begin{aligned} & \int d^3 \mathbf{x} \frac{\partial}{\partial \mathbf{x}} \cdot \mathbf{v} (n \bar{f}) + \frac{\mathbf{F}_{\text{ext}}}{m} \cdot \frac{\partial}{\partial \mathbf{v}} \bar{f} \\ &= \sum_k n_k \int d^3 \mathbf{V} \int d\sigma_k |\mathbf{v} - \mathbf{V}| \\ & \quad \times [\bar{f}(\mathbf{v} + \Delta \mathbf{v}; \mathbf{x}, t) \bar{F}_k(\mathbf{V} + \Delta \mathbf{V}; t) \\ & \quad - \bar{f}(\mathbf{v}; \mathbf{x}, t) \bar{F}_k(\mathbf{V}; t)] \end{aligned}$$

The 1st term on the R.H.S. is zero since it becomes a surface integral where $n=0$.

Combining this with the eq. on the left page yields

$$\left[\frac{\partial}{\partial t} + \langle \mathbf{v} \rangle \cdot \frac{\partial}{\partial \mathbf{x}} \right] n(\mathbf{x}; t) = 0$$

which implies a simple drift w/o diffusion, possible only if n is uniformly distributed.

Concept of Velocity Shell

Towards more realistic solutions to the B.Eq.

We will hence be forced to retain the time and position dependence in f_{bar} and think about another way of approximation.

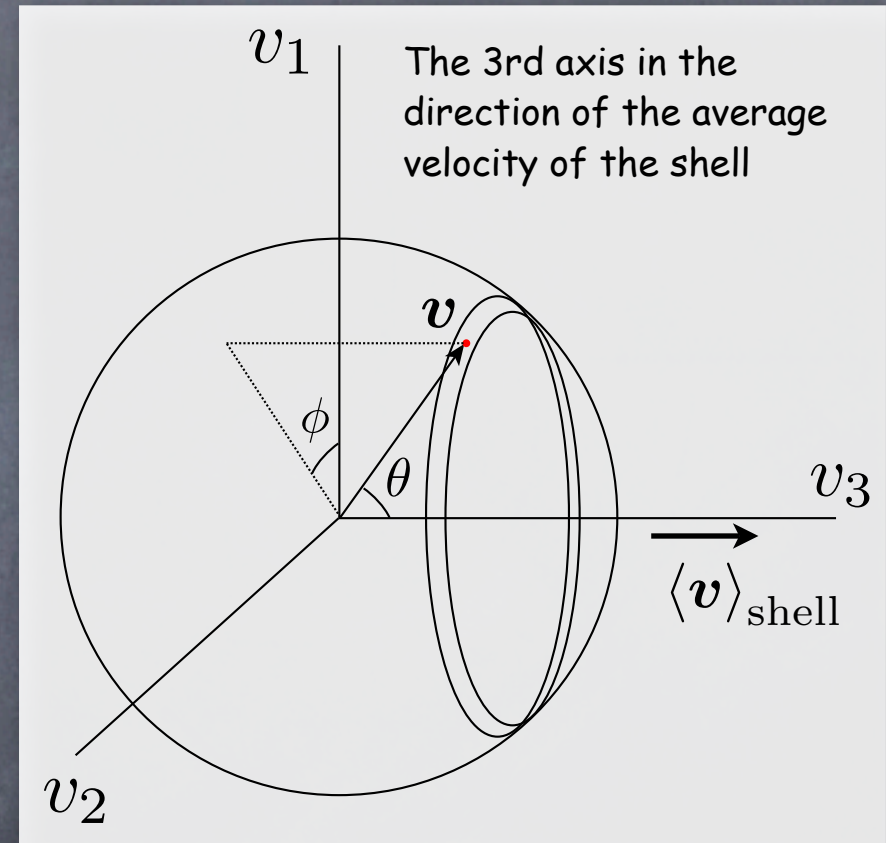
The Basic Idea

The motion of the electron is dominated by random and almost isotropic velocity with a small modulation (drift velocity) due to the external E and B fields.

The Velocity Shell

We hence consider a fraction of the phase space where the electron has speed in the range $(v, v+dv)$, a shell of a 3-dim sphere in the velocity space.

For the class of phase space points in the velocity shell, the distribution should be almost isotropic with the small modulation.



We will then consider the velocity space in a spherical coordinate system:

$$\Omega = (\cos \theta, \phi)$$

Harmonic Expansion

Expansion in terms of spherical harmonics

Harmonic Expansion

In each velocity shell, we expand \bar{f} in terms of spherical harmonics as

$$\bar{f}(\mathbf{v}; \mathbf{x}, t) = \sum_{l=0}^{\infty} \sum_{m=-l}^{m=+l} Y_l^m(\theta, \phi) \bar{f}_l^m(\mathbf{v}; \mathbf{x}, t)$$

The distribution will then be dominated by low l spherical harmonics,

$l=0$ (scalar=monopole) : dominant

$l=1$ (vector=dipole) : drift

Average shell velocity

$$\begin{aligned} \langle \mathbf{v} \rangle_{\Omega_v} &= \int d\Omega_v \mathbf{v} \bar{f}(\mathbf{v}; \mathbf{x}, t) / \int d\Omega_v \bar{f}(\mathbf{v}; \mathbf{x}, t) \\ &= \frac{v}{\sqrt{6} f_0^0} \begin{pmatrix} \bar{f}_1^{-1} - \bar{f}_1^1 \\ -i(\bar{f}_1^{-1} + \bar{f}_1^1) \\ \sqrt{2} \bar{f}_1^0 \end{pmatrix} \end{aligned}$$

Since we took the 3rd axis in the direction of the average velocity of the shell, this implies

$$\bar{f}_1^{-1} = \bar{f}_1^1 = 0$$

Ignoring $l>1$ terms, we can put

$$\begin{aligned} \bar{f}(\mathbf{v}; \mathbf{x}, t) &\approx f_0(\mathbf{v}; \mathbf{x}, t) + f_1(\mathbf{v}; \mathbf{x}, t) \cos \theta \\ &= f_0(\mathbf{v}; \mathbf{x}, t) + \mathbf{f}_1(\mathbf{v}; \mathbf{x}, t) \cdot \left(\frac{\mathbf{v}}{v} \right) \end{aligned}$$

where

$$\mathbf{f}_1(\mathbf{v}; \mathbf{x}, t) := \begin{pmatrix} 0 \\ 0 \\ f_1 \end{pmatrix}$$

The average shell velocity then becomes

$$\langle \mathbf{v} \rangle_{\Omega_v} = \frac{v \mathbf{f}_1}{3 f_0}$$

Notation

$$\langle l m | [\text{Object}] \rangle = \int d\Omega (Y_l^m)^* [\text{Object}]$$

Harmonic Expansion

Projection of B.Eq. to harmonic components

Harmonic Expansion of B.Eq.

All we need to do is to put

$$\begin{aligned}\bar{f}(\mathbf{v}; \mathbf{x}, t) &\approx f_0(\mathbf{v}; \mathbf{x}, t) + f_1(\mathbf{v}; \mathbf{x}, t) \cos \theta \\ &= f_0(\mathbf{v}; \mathbf{x}, t) + \mathbf{f}_1(\mathbf{v}; \mathbf{x}, t) \cdot \left(\frac{\mathbf{v}}{v}\right)\end{aligned}$$

into the Boltzmann equation, and project out $l=0$ (scalar) and $l=1$ (vector) components

$$\langle 00 | [\text{B.E.}] \rangle = \text{Scalar Eq.}$$

$$\langle 10 | [\text{B.E.}] \rangle = \text{Vector Eq.}$$

This projection is a tedious but doable mathematical exercise, at least for the L.H.S. of the Boltzmann equation. All you need to know is the composition rules of the spherical harmonics, which you must have learned in a Q.M. course.

I just show the results of the exercise.

The Scalar Equation ($l=0$)

$$\begin{aligned}\frac{\partial}{\partial t} (n f_0) + \frac{v}{3} \frac{\partial}{\partial \mathbf{x}} \cdot (n \mathbf{f}_1) + \frac{1}{4\pi v^2} \frac{\partial}{\partial v} \left[\frac{4\pi}{3} v^2 \frac{e\mathbf{E}}{m} \cdot n \mathbf{f}_1 \right] \\ = n \sum_k n_k \frac{1}{4\pi v^2} \frac{\partial}{\partial v} \bar{\sigma}_{m,k}(v; [f_0])\end{aligned}$$

where $\bar{\sigma}_{m,k}$ is in general a complicated fn. If collisions are all elastic, a concrete formula is known (c.f. Huxley & Crompton)

$$\begin{aligned}n n_k \bar{\sigma}_{m,k}(v; [f_0]) \\ = 4\pi v^2 n n_k v \underbrace{\sigma_{m,k}(v)}_{\text{effective collision frequency}} \left[\frac{m}{M_k} v f_0 + \frac{\langle V^2 \rangle}{3} \frac{\partial f_0}{\partial v} \right]\end{aligned}$$

effective collision frequency

$$\nu_{m,k} := n_k v \sigma_{m,k}(v)$$

The scalar equation can be interpreted as the continuity equation expressing energy conservation.

Harmonic Expansion

Projection of B.Eq. to harmonic components (continued)

Momentum Transfer X-Section

The collision term is characterized by a quantity called the momentum transfer cross section.

It is defined in general by

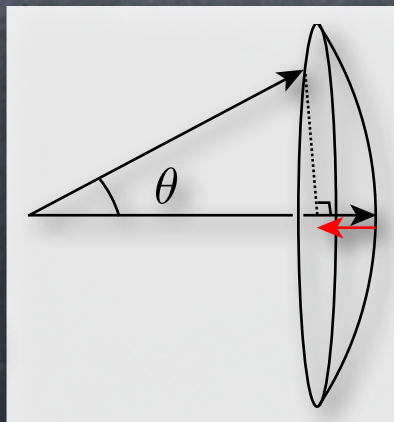
$$\sigma_{m,k} = \sigma_{0,k} - \frac{v_r'}{v_r} \sigma_{1,k}$$

where v_r and v_r' are relative speeds of electrons in the molecule rest frame before and after the collision, and their ratio is unity for elastic scattering, and

$$\sigma_{0,k} = \int d\sigma_k$$

$$\sigma_{1,k} = \int d\sigma_k \cos \theta$$

$$p \sigma_{m,k} = \int d\sigma_k p (1 - \cos \theta)$$



The Vector Equation (l=1)

$$\frac{\partial}{\partial t} (n \mathbf{f}_1) + v \frac{\partial}{\partial x} (n f_0) + \frac{e \mathbf{E}}{m} \frac{\partial}{\partial v} (n f_0) - \boldsymbol{\omega} \times (n \mathbf{f}_1) = -\bar{\nu}_m(v) (n \mathbf{f}_1)$$

where

$$\bar{\nu}_m := \sum_k n_k v \sigma_{m,k}(v) : \text{effective coll. freq.}$$

$$\boldsymbol{\omega} := \frac{(-e) \mathbf{B}}{mc} : \text{cyclotron freq. vec.}$$

Notice that the electron charge is -ve, hence (-e) is +ve.

The vector equation can be interpreted as the continuity equation expressing momentum conservation.

Vector Equation

Interpretation of Vector Eq.

The effective collision frequency is related to mean free time

$$\tau = \frac{1}{\bar{\nu}_m}$$

On the other hand the total momentum of the velocity shell ($v, v+dv$) is

$$dp_{tot} = (4\pi v^2 dv) (n f_0) m \frac{v f_1}{3 f_0} = \frac{4\pi v^2 dv}{3} m v (n f_1)$$

Multiplying the both sides of the vector eq. by tau with this in mind makes the meanings of the vector eq. clearer.

This part remains even after the steady state is reached and hence should be kept as significant.

Quickly become small after injection

$$\tau \frac{\partial}{\partial t} (n f_1)$$

change of distribution during tau

path length

$$(\tau v) \frac{\partial}{\partial x} (n f_0)$$

Can be large for a point source

velocity increase during tau

velocity change by a single collision

$$\left(\tau \frac{e \mathbf{E}}{m} \right) \frac{\partial}{\partial v} (n f_0) - (\boldsymbol{\omega} \tau) \times (n \mathbf{f}_1) = - (n \mathbf{f}_1)$$

rotation during tau

Vector Equation

Separation of Drift and Diffusion

The Vector Equation

$$\begin{aligned} \cancel{\frac{\partial}{\partial t} (n \mathbf{f}_1)} + v \frac{\partial}{\partial \mathbf{x}} (n f_0) + \frac{e \mathbf{E}}{m} \frac{\partial}{\partial v} (n f_0) - \boldsymbol{\omega} \times (n \mathbf{f}_1) \\ = -\bar{v}_m(v) (n \mathbf{f}_1) \end{aligned}$$

We assume that the 1st term (t-derivative) is negligible compared with the rest. This assumption implies that the electron is in a quasi-equilibrium at least locally.

Then we have

$$\begin{aligned} v \frac{\partial}{\partial \mathbf{x}} (n f_0) + \frac{e \mathbf{E}}{m} \frac{\partial}{\partial v} (n f_0) - \boldsymbol{\omega} \times (n \mathbf{f}_1) \\ \approx -\bar{v}_m(v) (n \mathbf{f}_1) \end{aligned}$$

We now decompose \mathbf{f}_1 as

$$\mathbf{f}_1 = \mathbf{f}_E + \mathbf{f}_G$$

to separate the vector eq. into the following two:

$$\bar{v}_m(v) (n \mathbf{f}_E) - \boldsymbol{\omega} \times (n \mathbf{f}_E) = -\frac{e \mathbf{E}}{m} \frac{\partial}{\partial v} (n f_0)$$

$$\bar{v}_m(v) (n \mathbf{f}_G) - \boldsymbol{\omega} \times (n \mathbf{f}_G) = -v \frac{\partial}{\partial \mathbf{x}} (n f_0)$$

Notice that these are linear equations of the form

$$[\bar{v}_m(v) - \boldsymbol{\omega} \times] (n \mathbf{f}_{E/G}) = [\text{fn. of } f_0]$$

that can be solved by matrix inversion,

$$(n \mathbf{f}_{E/G}) = [\bar{v}_m(v) - \boldsymbol{\omega} \times]^{-1} [\text{fn. of } f_0]$$

once f_0 is given.

Notice also that upon the integration over \mathbf{x} the contribution from \mathbf{f}_G must vanish.

$$\begin{aligned} & [\bar{v}_m(v) - \boldsymbol{\omega} \times] \int d^3 \mathbf{x} (n \mathbf{f}_G) \\ & = -v \int d^3 \mathbf{x} \frac{\partial}{\partial \mathbf{x}} (n \mathbf{f}_G) \\ & = \text{Surf. int.} = 0 \end{aligned}$$

Vector Equation

Separation of Drift and Diffusion

Now recall that f_1 is related to the drift velocity of the shell through

$$\langle \mathbf{v} \rangle_{\Omega_v} = \frac{v \mathbf{f}_1}{3f_0}$$

We can hence rewrite the average velocity of the shell as

$$\langle \mathbf{v} \rangle_{\Omega_v} =: \mathbf{W} = \mathbf{W}_E + \mathbf{W}_G$$

with

$$\mathbf{W}_{E/G} := \frac{v \mathbf{f}_{E/G}}{3f_0}$$

Notice that \mathbf{W} is a function of the speed v and the position of the electron, and the average over the whole phase space sample is given by

$$\begin{aligned} \langle \mathbf{v} \rangle &= \int d^3 \mathbf{x} \int (4\pi) v^2 dv (n f_0) \mathbf{W} \\ &= \int \left(\frac{4\pi}{3} \right) v^3 dv \int d^3 \mathbf{x} (n f_1) \end{aligned}$$

This means that the f_G and hence \mathbf{W}_G does not contribute to the average velocity of the whole ensemble:

$$\langle \mathbf{v} \rangle = \langle \mathbf{W}_E \rangle$$

and

$$\langle \mathbf{W}_G \rangle = 0$$

We can hence interpret \mathbf{W}_E as the drift velocity due to the external field and \mathbf{W}_G as the convection velocity due to diffusion of the velocity shell at a given spatial point.

We will hence concentrate on \mathbf{W}_E for our discussions on the drift velocity v_D , while for our discussions on the diffusion we will focus on \mathbf{W}_G , which is our next task.

Drift Velocity

Mobility Matrix

We start from the equation for $f\mathbf{E}$, which can be rewritten with \mathbf{W}_E as

$$f_0 [\bar{v}_m(v) - \boldsymbol{\omega} \times] \mathbf{W}_E = -\frac{v}{3} \left(\frac{\partial}{\partial v} f_0 \right) \frac{e \mathbf{E}}{m}$$

Notice that $n(\mathbf{x}; t)$ does not depend on v and hence can be cancelled out.

We now introduce a matrix $[\mathbf{M}]$:

$$\begin{aligned} [\mathbf{M}] &:= [\bar{v}_m(v) - \boldsymbol{\omega} \times] \\ &= \begin{pmatrix} \nu & \omega_3 & -\omega_2 \\ -\omega_3 & \nu & \omega_1 \\ \omega_2 & -\omega_1 & \nu \end{pmatrix} \end{aligned}$$

where use has been made of a shorthand:

$$\bar{v}_m(v) \rightarrow \nu$$

For notational convenience, we will use this abbreviation in what follows.

Now all we need to do is a matrix inversion.

Recall your linear algebra course, then the reciprocal of the matrix \mathbf{M} is given by

$$[\mathbf{M}]^{-1} = \begin{pmatrix} \nu^2 + \omega_1^2 & \omega_1\omega_2 - \nu\omega_3 & \omega_1\omega_3 + \nu\omega_2 \\ \omega_2\omega_1 + \nu\omega_3 & \nu^2 + \omega_2^2 & \omega_2\omega_3 - \nu\omega_1 \\ \omega_3\omega_1 - \nu\omega_2 & \omega_3\omega_2 + \nu\omega_1 & \nu^2 + \omega_3^2 \end{pmatrix} \div \frac{\nu(\nu^2 + \omega^2)}{\det[\mathbf{M}]}$$

with

$$\omega^2 := \omega^2 = \omega_1^2 + \omega_2^2 + \omega_3^2$$

and

$$\boldsymbol{\omega} := \frac{(-e)\mathbf{B}}{mc}$$

\mathbf{W}_E can now be written as

$$f_0 \mathbf{W}_E = -\frac{v}{3} \left(\frac{\partial}{\partial v} f_0 \right) [\mathbf{M}]^{-1} \left(\frac{e \mathbf{E}}{m} \right)$$

which can be averaged over v to give

$$\begin{aligned} \langle \mathbf{W}_E \rangle_v(\mathbf{x}; t) &:= \int (4\pi)v^2 dv f_0 \mathbf{W}_E \\ &= [\boldsymbol{\mu}] \mathbf{E} \end{aligned}$$

Drift Velocity

Mobility Matrix (continued)

The Mobility Matrix

We introduced the local mobility matrix:

$$[\mu] := -\frac{4\pi e}{3m} \int dv v^3 \left(\frac{\partial}{\partial v} f_0 \right) [M]^{-1}$$

which is in general a function of $(\mathbf{x}; t)$.

To get the position-averaged mobility suitable for the centroid motion, we define

$$f_0^*(v; t) := \int d^3x (n f_0)$$

and the (global) mobility matrix:

$$[\mu^*] := -\frac{4\pi e}{3m} \int dv v^3 \left(\frac{d}{dv} f_0^* \right) [M]^{-1}$$

With this, we can write

$$\langle \mathbf{W} \rangle = \langle \mathbf{W}_E \rangle = [\mu^*] \mathbf{E}$$

Notice that the mobility matrix is proportional to a unit matrix if $B=0$.

If there is a B-field, the mobility matrix will acquire nonzero off-diagonal elements and hence the direction of the E-field and the direction of the drift velocity will differ (so-called Lorentz angle effects).

Special Case [1] ($B=0$)

The matrix $[M]$ becomes "nu" and hence the $[\mu^*]$ becomes a single number:

$$\mu^* = -\frac{4\pi e}{3m} \int_0^\infty dv \frac{v^3}{v} \left(\frac{d}{dv} f_0^* \right)$$

The drift direction should be anti-parallel with the E-field. This suggests that the integral should be negative, since $(e < 0)$. Assuming that f_0^* has a single peak, and the integral weights more on the higher side of the peak, it is indeed so.

Drift Velocity

Mobility Matrix (continued)

Special Case [2] (B//E)

This is the case of our interest. Assuming that E and B are in the 3-axis direction, then

$$\omega = \begin{pmatrix} 0 \\ 0 \\ \omega \end{pmatrix}$$

and the inverse of [M] becomes

$$[M]^{-1} = \frac{1}{\nu(\nu^2 + \omega^2)} \begin{pmatrix} \nu^2 & -\nu\omega & 0 \\ \nu\omega & \nu^2 & 0 \\ 0 & 0 & \nu^2 + \omega^2 \end{pmatrix}$$

But the E-field has no 1- or 2- components, there will be no 1- or 2-components in the drift velocity, either. Moreover, the 3rd component coincides with the B=0 case. There is hence no B-field effect on the drift velocity in the E//B case.

Special Case [3] (v-dist=delta fn.)

If the velocity distribution can be taken as a delta function:

$$f_0^* = \frac{1}{4\pi v^2} \delta(v - \bar{v})$$

Putting this into the def. of the mobility matrix, we have

$$\begin{aligned} [\mu^*] &= -\frac{4\pi e}{3m} \int dv v^3 \left(\frac{d}{dv} f_0^* \right) [M]^{-1} \\ &= -\frac{4\pi e}{3m} [M]^{-1}(\bar{v}) \int dv \left[\frac{d}{dv} (v^3 f_0^*) - \frac{d}{dv} (v^3) f_0^* \right] \\ &= \frac{4\pi e}{m} [M]^{-1}(\bar{v}) \int dv v^2 f_0^* = \frac{e}{m} [M]^{-1}(\bar{v}) \end{aligned}$$

The mobility matrix is thus parameterized by just two parameters, the collision freq. at \bar{v} and the cyclotron frequency.

Mean Free Time

Mobility Matrix (continued)

Usual Simplistic Arguments

Case (3) formula is usually obtained by time-averaging the Newtonian equation of motion.

$$m \frac{d\mathbf{v}}{dt} = e \left[\mathbf{E} + \frac{\mathbf{v}}{c} \times \mathbf{B} \right] + \mathbf{F}_{\text{coll}}$$

We define the time average of a variable A to be

$$\langle A \rangle_t := \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T dt A(t)$$

Upon this time average, the L.H.S. of the Newtonian eq. vanishes, since we are considering a bounded motion for which the velocity stays finite. We hence have

$$0 = e \left[\mathbf{E} + \frac{\langle \mathbf{v} \rangle_t}{c} \times \mathbf{B} \right] + \langle \mathbf{F}_{\text{coll}} \rangle_t$$

We now need to evaluate the time average of the collision force:

$$\begin{aligned} \langle \mathbf{F}_{\text{coll}} \rangle_t &= \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T dt \mathbf{F}_{\text{coll}} \\ &= \lim_{N \rightarrow \infty} \frac{1}{\sum_{i=1}^N \Delta T_i} \sum_{i=1}^N \int_{t_{i-1}}^{t_i} dt \mathbf{F}_{\text{coll}}(t) \\ &= \lim_{N \rightarrow \infty} \frac{1}{\sum_{i=1}^N \Delta T_i / N} \frac{1}{N} \sum_{i=1}^N \int_{t_i - \frac{\delta t}{2}}^{t_i + \frac{\delta t}{2}} dt \mathbf{F}_{\text{coll}}(t) \\ &= \frac{1}{\tau} \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{i=1}^N m \Delta \mathbf{v} = \frac{1}{\tau} \langle m \Delta \mathbf{v} \rangle \end{aligned}$$

Notice that there appears the mean free time and the average momentum transfer. The momentum transfer averaged over all angles is easy to get for isotropic collisions

$$\begin{aligned} \langle m \Delta \mathbf{v} \rangle_{\Omega} &= \int \frac{d\Omega}{4\pi} m \Delta \mathbf{v} \\ &= - \int \frac{d \cos \theta}{2} m \mathbf{v} (1 - \cos \theta) = -m \mathbf{v} \end{aligned}$$

Mean Free Time

Mobility Matrix (continued)

We can think of the average that appears in

$$\langle \mathbf{F}_{\text{coll}} \rangle_t = \frac{1}{\tau} \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{i=1}^N m \Delta \mathbf{v} = \frac{1}{\tau} \langle m \Delta \mathbf{v} \rangle$$

being first taken over scattering angles for each group with nearly the same momentum and then over such groups. Then we have

$$\langle \mathbf{F}_{\text{coll}} \rangle_t = -\frac{1}{\tau} m \langle \mathbf{v} \rangle$$

Collecting things together, we arrive at the time-averaged Langevin equation:

$$\left[\frac{1}{\tau} - \frac{(-e)\mathbf{B}}{mc} \times \right] \langle \mathbf{v} \rangle = \frac{e\mathbf{E}}{m}$$

Notice that $1/\tau = \nu$ and

$$\omega := \frac{(-e)\mathbf{B}}{mc}$$

tell us that the content of the square bracket is the same $[M]$ we met before.

The Drift Velocity Formula

This is a simple linear equation, and can be solved by matrix inversion as we did, and yields the formula you often see in the text book

$$\langle \mathbf{v} \rangle = \left(\frac{\mu E}{1 + (\omega\tau)^2} \right) \left(\hat{\mathbf{E}} + (\omega\tau) [\hat{\mathbf{E}} \times \hat{\mathbf{B}}] + (\omega\tau)^2 (\hat{\mathbf{E}} \cdot \hat{\mathbf{B}}) \hat{\mathbf{B}} \right)$$

This formula can hence be regarded as the limiting case of the delta function like \mathbf{v} distribution.

We can also rewrite the Langevin equation in the following form

$$[1 - \omega\tau \times] \langle \mathbf{v} \rangle = \frac{e\tau}{m} \mathbf{E}$$

This implies

$$[1 - \omega\tau \times] \langle \mathbf{v} \rangle \cdot \langle \hat{\mathbf{v}} \rangle = |\langle \mathbf{v} \rangle| = \frac{e\tau}{m} \mathbf{E} \cdot \langle \hat{\mathbf{v}} \rangle$$

which is known as Tonk's theorem.

Diffusion

Diffusion Tensor

So far we have been discussing WE (or equivalently fE), the drift due to the external fields.

We now turn our attention to the vector eq. for WG (fG), which can be cast into the form:

$$(n f_0) [\bar{v}_m(v) - \boldsymbol{\omega} \times] \mathbf{W}_G = -\frac{v^2}{3} \left(\frac{\partial}{\partial x} (n f_0) \right)$$

Notice that this time, since $n(x;t)$ depends on x , we cannot cancel out n . Nevertheless, there appears the same matrix $[M]$:

$$\begin{aligned} [M] &:= [\bar{v}_m(v) - \boldsymbol{\omega} \times] \mathbf{W}_E \\ &= \begin{pmatrix} \nu & \omega_3 & -\omega_2 \\ -\omega_3 & \nu & \omega_1 \\ \omega_2 & -\omega_1 & \nu \end{pmatrix} \end{aligned}$$

and hence with the same inverse matrix:

$$[M]^{-1} = \begin{pmatrix} \nu^2 + \omega_1^2 & \omega_1\omega_2 - \nu\omega_3 & \omega_1\omega_3 + \nu\omega_2 \\ \omega_2\omega_1 + \nu\omega_3 & \nu^2 + \omega_2^2 & \omega_2\omega_3 - \nu\omega_1 \\ \omega_3\omega_1 - \nu\omega_2 & \omega_3\omega_2 + \nu\omega_1 & \nu^2 + \omega_3^2 \end{pmatrix} \div \frac{\nu(\nu^2 + \omega^2)}{\det [M]}$$

with

$$\omega^2 := \boldsymbol{\omega}^2 = \omega_1^2 + \omega_2^2 + \omega_3^2$$

and

$$\boldsymbol{\omega} := \frac{(-e)\mathbf{B}}{mc}$$

The solution is then

$$(n f_0) \mathbf{W}_G = -\frac{v^2}{3} [M]^{-1} \left(\frac{\partial}{\partial x} (n f_0) \right)$$

which can be averaged over v to give

$$\begin{aligned} n \langle \mathbf{W}_G \rangle (\mathbf{x}; t) &:= \int (4\pi)v^2 dv (n f_0) \mathbf{W}_G \\ &= -\frac{4\pi}{3} \int v^2 dv v^2 [M]^{-1} \left(\frac{\partial}{\partial x} (n f_0) \right) \end{aligned}$$

Diffusion

Diffusion Matrix

Crucial step is to replace f_0 on the R.H.S. by f_0^* :

$$f_0^*(v; t) := \int d^3x (n f_0)$$

so that we can take out f_0^* out of the spatial derivative and get

$$n \langle \mathbf{W}_G \rangle_v = - [D] \frac{\partial}{\partial \mathbf{x}} n$$

with the diffusion matrix $[D]$ given by

$$[D] = \frac{4\pi}{3} \int v^2 dv v^2 [M]^{-1} f_0^*$$

The inverse of $[M]$ is as before:

$$[M]^{-1} = \begin{pmatrix} \nu^2 + \omega_1^2 & \omega_1 \omega_2 - \nu \omega_3 & \omega_1 \omega_3 + \nu \omega_2 \\ \omega_2 \omega_1 + \nu \omega_3 & \nu^2 + \omega_2^2 & \omega_2 \omega_3 - \nu \omega_1 \\ \omega_3 \omega_1 - \nu \omega_2 & \omega_3 \omega_2 + \nu \omega_1 & \nu^2 + \omega_3^2 \end{pmatrix} \\ \div \nu (\nu^2 + \omega^2) \\ \det [M]$$

with

$$\omega^2 := \omega^2 = \omega_1^2 + \omega_2^2 + \omega_3^2$$

and

$$\omega := \frac{(-e)B}{mc}$$

The approximation

$$\frac{\partial}{\partial \mathbf{x}} (n f_0) \approx f_0^* \frac{\partial}{\partial \mathbf{x}} (n)$$

allowed us to define the diffusion matrix $[D]$ that satisfies the usual definition

$$\underbrace{n \langle \mathbf{W}_G \rangle_v}_{\vdots} = - [D] \underbrace{\frac{\partial}{\partial \mathbf{x}} n}_{\vdots}$$

current density

(w/o common drift)

grad (density)

There is some subtlety in this approx. but we will not get into it.

Diffusion

Diffusion Matrix (continued)

Special Case [1] (B=0)

The matrix [M] becomes "nu" and hence the [D] becomes a single number:

$$D = \frac{4\pi}{3} \int dv \frac{v^4}{\nu} f_0^*(v)$$

where the collision frequency is given by

$$\nu = \sum_k n_k v \sigma_{m,k}(v)$$

We can hence rewrite the diffusion constant as

$$D = \frac{1}{3} \int dv \frac{(4\pi v^2) f_0^*(v)}{\sum_k n_k v \sigma_{m,k}(v)} v^2$$

The diffusion is hence isotropic (as long as the approximation is valid) and inversely proportional to gas density and X-section.

Special Case [2] (B//E)

This is the case of our interest. Assuming that E and B are in the 3-axis direction, then

$$\omega = \begin{pmatrix} 0 \\ 0 \\ \omega \end{pmatrix}$$

and the inverse of [M] becomes

$$[M]^{-1} = \frac{1}{\nu(\nu^2 + \omega^2)} \begin{pmatrix} \nu^2 & -\nu\omega & 0 \\ \nu\omega & \nu^2 & 0 \\ 0 & 0 & \nu^2 + \omega^2 \end{pmatrix}$$

Then we have

$$D_L = \frac{1}{3} \int dv \frac{(4\pi v^2) f_0^*(v)}{\nu} v^2 = D_{33}$$

$$D_T = \frac{1}{3} \int dv \frac{(4\pi v^2) f_0^*(v) \nu}{\nu^2 + \omega^2} v^2 = D_{11,22}$$

$$D_{12} = -D_{21} = \frac{1}{3} \int dv \frac{(4\pi v^2) f_0^*(v) \omega}{\nu^2 + \omega^2} v^2$$

All the other components are zero.

Diffusion

Diffusion Matrix (continued)

Notice that the longitudinal diffusion const.

$$D_L = \frac{1}{3} \int dv \frac{(4\pi v^2) f_0^*(v)}{\nu} v^2 = D_{33}$$

is the same as with the $B=0$ case.

On the other hand, the transverse one

$$D_T = \frac{1}{3} \int dv \frac{(4\pi v^2) f_0^*(v) \nu}{\nu^2 + \omega^2} v^2 = D_{11,22}$$

is reduced by a factor

$$\frac{\nu^2}{\nu^2 + \omega^2} = \frac{1}{1 + (\omega\tau)^2} \quad \text{with} \quad \tau = \frac{1}{\nu}$$

in the integrand. Where the tau, being the inverse of the collision frequency, is the mean free time between collisions.

$$D_{12} = -D_{21} = \frac{1}{3} \int dv \frac{(4\pi v^2) f_0^*(v) \omega}{\nu^2 + \omega^2} v^2$$

corresponds to rotation about the field axis but it is not of our interest.

Special Case [3] (v -dist=delta fn.)

If the velocity distribution can be taken as a delta function:

$$f_0^* = \frac{1}{4\pi v^2} \delta(v - \bar{v})$$

Putting this into the def. of the diffusion matrix:

$$[D] = \frac{4\pi}{3} \int v^2 dv v^2 [M]^{-1} f_0^*$$

with the inverse of $[M]$ given by

$$[M]^{-1} = \begin{pmatrix} \nu^2 + \omega_1^2 & \omega_1\omega_2 - \nu\omega_3 & \omega_1\omega_3 + \nu\omega_2 \\ \omega_2\omega_1 + \nu\omega_3 & \nu^2 + \omega_2^2 & \omega_2\omega_3 - \nu\omega_1 \\ \omega_3\omega_1 - \nu\omega_2 & \omega_3\omega_2 + \nu\omega_1 & \nu^2 + \omega_3^2 \end{pmatrix} \div \nu (\nu^2 + \omega^2)$$

we have

$$[D] = \frac{1}{3} \bar{v}^2 [M]^{-1}(\bar{v})$$

If $B=0$, this implies a naive expectation

$$[D] = \frac{1}{3} \bar{v}^2 \tau = \frac{1}{3} \frac{(\bar{v}\tau)^2}{\tau}$$

Scalar Equation

We need to solve the scalar equation, too

What We Have Done So Far

a) We have shown that

$$\langle \mathbf{W}_G \rangle = 0 \quad \text{and, hence} \quad \langle \mathbf{v} \rangle = \langle \mathbf{W}_E \rangle$$

which means diffusion does not contribute to the drift velocity of the centroid, as naively expected.

b) We have defined the mobility matrix for the centroid

$$[\mu^*] := -\frac{4\pi e}{3m} \int dv v^3 \left(\frac{d}{dv} f_0^* \right) [M]^{-1}$$

$$[M]^{-1} = \begin{pmatrix} \nu^2 + \omega_1^2 & \omega_1\omega_2 - \nu\omega_3 & \omega_1\omega_3 + \nu\omega_2 \\ \omega_2\omega_1 + \nu\omega_3 & \nu^2 + \omega_2^2 & \omega_2\omega_3 - \nu\omega_1 \\ \omega_3\omega_1 - \nu\omega_2 & \omega_3\omega_2 + \nu\omega_1 & \nu^2 + \omega_3^2 \end{pmatrix} \div \nu (\nu^2 + \omega^2)$$

with which, we can write

$$\langle \mathbf{W} \rangle = \langle \mathbf{W}_E \rangle = [\mu^*] \mathbf{E}$$

c) We have also defined the diffusion matrix

$$[D] = \frac{4\pi}{3} \int v^2 dv v^2 [M]^{-1} f_0^*$$

with which the convection current due to diffusion is given by

$$n \langle \mathbf{W}_G \rangle_v = -[D] \frac{\partial}{\partial \mathbf{x}} n$$

These results came solely from the vector equation, and f_0^* remains as unknown.

Remaining Questions

a) How should we relate $[D]$ to the electron cloud size? In other words, we need to know the spatial distribution, $n(\mathbf{x};t)$.

b) How can we determine f_0^* ?

In order to answer these questions, we now need to look at the scalar equation.

Scalar Equation

Derivation of Diffusion Equation

The Diffusion Equation

We hence start from the scalar equation

$$\begin{aligned} \frac{\partial}{\partial t} (n f_0) + \frac{v}{3} \frac{\partial}{\partial x} \cdot (n \mathbf{f}_1) + \frac{1}{4\pi v^2} \frac{\partial}{\partial v} \left[\frac{4\pi}{3} v^2 \frac{e\mathbf{E}}{m} \cdot n \mathbf{f}_1 \right] \\ = n \sum_k n_k \frac{1}{4\pi v^2} \frac{\partial}{\partial v} \bar{\sigma}_{m,k}(v; [f_0]) \end{aligned}$$

By defining

$$\sigma_E := \frac{4\pi}{3} v^2 \frac{e\mathbf{E}}{m} \cdot n \mathbf{f}_1$$

and

$$\sigma_{\text{coll}} := \sum_k n_k \bar{\sigma}_{m,k}$$

we can rewrite it in the following form

$$\frac{\partial}{\partial t} (n f_0) + \frac{v}{3} \frac{\partial}{\partial x} \cdot (n \mathbf{f}_1) = -\frac{1}{4\pi v^2} \frac{\partial}{\partial v} (\sigma_E - \sigma_{\text{coll}})$$

Recalling

$$\int d^3 \mathbf{v} f_0 = \int (4\pi v^2) dv f_0 = 1$$

$$f_0^*(v; t) := \int d^3 \mathbf{x} (n f_0)$$

we v-integrate the both sides to get

$$\frac{\partial}{\partial t} n + \frac{\partial}{\partial x} \cdot \left(n \int (4\pi v^2) dv f_0 \frac{v \mathbf{f}_1}{3 f_0} \right) = 0$$

where the R.H.S. is a surface integral.

Recall also the shell averaged velocity formula

$$\langle \mathbf{v} \rangle_{\Omega_v} = \frac{v \mathbf{f}_1}{3 f_0}$$

then the quantity in the parentheses is the current density at $(\mathbf{x}; t)$

$$n \int (4\pi v^2) dv f_0 \frac{v \mathbf{f}_1}{3 f_0} = n \langle \mathbf{W} \rangle_v$$

The above equation now becomes

$$\frac{\partial}{\partial t} n + \frac{\partial}{\partial x} (n \langle \mathbf{W} \rangle_v) = 0$$

which is none other than the usual equation of continuity.

Scalar Equation

Derivation of Diffusion Equation

In to this continuity equation:

$$\frac{\partial}{\partial t} n + \frac{\partial}{\partial x} (n \langle \mathbf{W} \rangle_v) = 0$$

we can now put

$$n \langle \mathbf{W} \rangle_v = n \langle \mathbf{W}_E \rangle_v + n \langle \mathbf{W}_G \rangle_v$$

recalling

$$\langle \mathbf{W}_E \rangle_v = [\mu] \mathbf{E} \approx [\mu^*] \mathbf{E} = \langle v \rangle$$

and

$$n \langle \mathbf{W}_G \rangle_v = -[D] \frac{\partial}{\partial x} n$$

We then obtain

$$\frac{\partial}{\partial t} n + \langle v \rangle \cdot \frac{\partial}{\partial x} n - \left(\frac{\partial}{\partial x} \right)^T [D] \left(\frac{\partial}{\partial x} \right) n = 0$$

which is none other than the diffusion eq. as you transform this into a more familiar form if [D] is a constant D times a unit matrix

$$\frac{\partial}{\partial t} n + \langle v \rangle \cdot \frac{\partial}{\partial x} n - D \left(\frac{\partial}{\partial x} \right)^2 n = 0$$

In the co-moving frame of the centroid ($x' = x - \langle v \rangle t$), this becomes

$$\frac{\partial}{\partial t} n - D \left(\frac{\partial}{\partial x'} \right)^2 n = 0$$

The solution to this equation with the point source initial condition is given by

$$n = \left(\frac{1}{\sqrt{2\pi(2Dt)}} \right)^3 \exp \left[-\frac{x'^2}{2(2Dt)} \right]$$

This implies that the electron cloud will have a Gaussian spread given by

$$\sigma_x^2 = 2Dt$$

after created as a point-like cluster.

OK, now the remaining task is f0*!

Scalar Equation

Equation for f_0^*

Velocity Distribution Function

We again start from the scalar equation

$$\frac{\partial}{\partial t} (n f_0) + \frac{v}{3} \frac{\partial}{\partial x} \cdot (n f_1) = -\frac{1}{4\pi v^2} \frac{\partial}{\partial v} (\sigma_E - \sigma_{\text{coll}})$$

This time we integrate out x , since we are now interested in the velocity distribution

$$f_0^*(v; t) := \int d^3x (n f_0)$$

Upon this integration the 2nd term of the L.H.S. vanishes since it becomes a surface integral where the electron is absent.

Noting that the R.H.S. is a function of f_0 and this spatial integration replaces f_0 by f_0^* , we have

$$\frac{\partial}{\partial t} f_0^* = -\frac{1}{4\pi v^2} \frac{\partial}{\partial v} (\sigma_E^* - \sigma_{\text{coll}}^*)$$

Ignoring the time derivative assuming that the electron's velocity distribution reaches a steady state in a short time, this reads

$$0 = -\frac{1}{4\pi v^2} \frac{\partial}{\partial v} (\sigma_E^* - \sigma_{\text{coll}}^*)$$

The equation expresses the balance between the external force and the collision force. The concrete form of the collision term depends on the nature of the molecules in the gas in question and hence the concrete form of the equation also depends on it. When only elastic collision is there, it is known (c.f. Huxley & Crompton) that the equation becomes

$$(u^2 + \langle V^2 \rangle) \frac{d}{dv} f_0^* + \frac{3mv}{M} f_0^* = 0$$

with

$$u := \frac{eE'}{m\nu} = \frac{eE'}{m} \tau$$

Scalar Equation

Solution for f_0^* (elastic only case)

Solution for f_0^*

The equation for f_0^* for a monatomic gas and for elastic collisions only

$$(u^2 + \langle V^2 \rangle) \frac{d}{dv} f_0^* + \frac{3mv}{M} f_0^* = 0$$

with

$$u := \frac{eE}{m\nu} = \frac{eE}{m} \tau$$

has the solution

$$f_0^*(v) = A \exp \left[-\frac{3m}{M} \int_0^v \frac{v' dv'}{u^2 + \langle V^2 \rangle} \right]$$

Special Case I ($E=0$)

In this case $u=0$, and since

$$\left\langle \frac{1}{2} M V^2 \right\rangle = \frac{3}{2} k_B T$$

we end up with

$$f_0^*(v) = A \exp \left[-\frac{m v^2 / 2}{k_B T} \right]$$

which is none other than the Maxwellian distribution as expected.

Special Case II ($\nu/v = \text{const.}$)

When the collision frequency divided by v or equivalently the cross section can be regarded as constant within the range where f_0^* is significant, we have instead

$$f_0^*(v) = A \exp \left[-\left(\frac{v}{\alpha} \right)^4 \right]$$

with

$$\alpha^4 = \frac{4M}{3m} \left(\frac{eE/n_M}{m \sigma_m} \right)^2$$

This is called a Druyvesteyn distribution and has a sharper peak than the Maxwellian.

Cross Section Shape

How σ_m behaves?

Order of Magnitude Estimate

The most popular chamber gas is Ar, so let's try an order of magnitude estimation of the electron-Ar cross section.

Ar has an atomic number $A=18$ with the first 3 shells filled up. It's a perfectly symmetric molecule and hence the remnant electric field dies away very quickly. The scattering cross section is therefore largely determined by the size of the outermost orbit. The electron in the outermost orbit experiences the attractive force from the nucleus largely shielded by the other electrons.

Let's assume that because of this shielding, the electron only feels the net charge of 1 unit of $(-e)$.

The orbit radius can then be approximated as exactly as with a hydrogen atom for $n=3$.

$$\begin{aligned}r(n) &\simeq \frac{\hbar}{mc\alpha_{\text{QED}}} n \\&\simeq (0.5 \times 10^{-8} [\text{cm}]) \times 3 \\&= 1.5 \times 10^{-8} [\text{cm}] \\ \sigma_{\text{Ar}} &\simeq \pi r(3)^2 \\&\simeq \pi (1.5 \times 10^{-8} [\text{cm}])^2 \\&= 7.1 \times 10^{-16} [\text{cm}^2]\end{aligned}$$

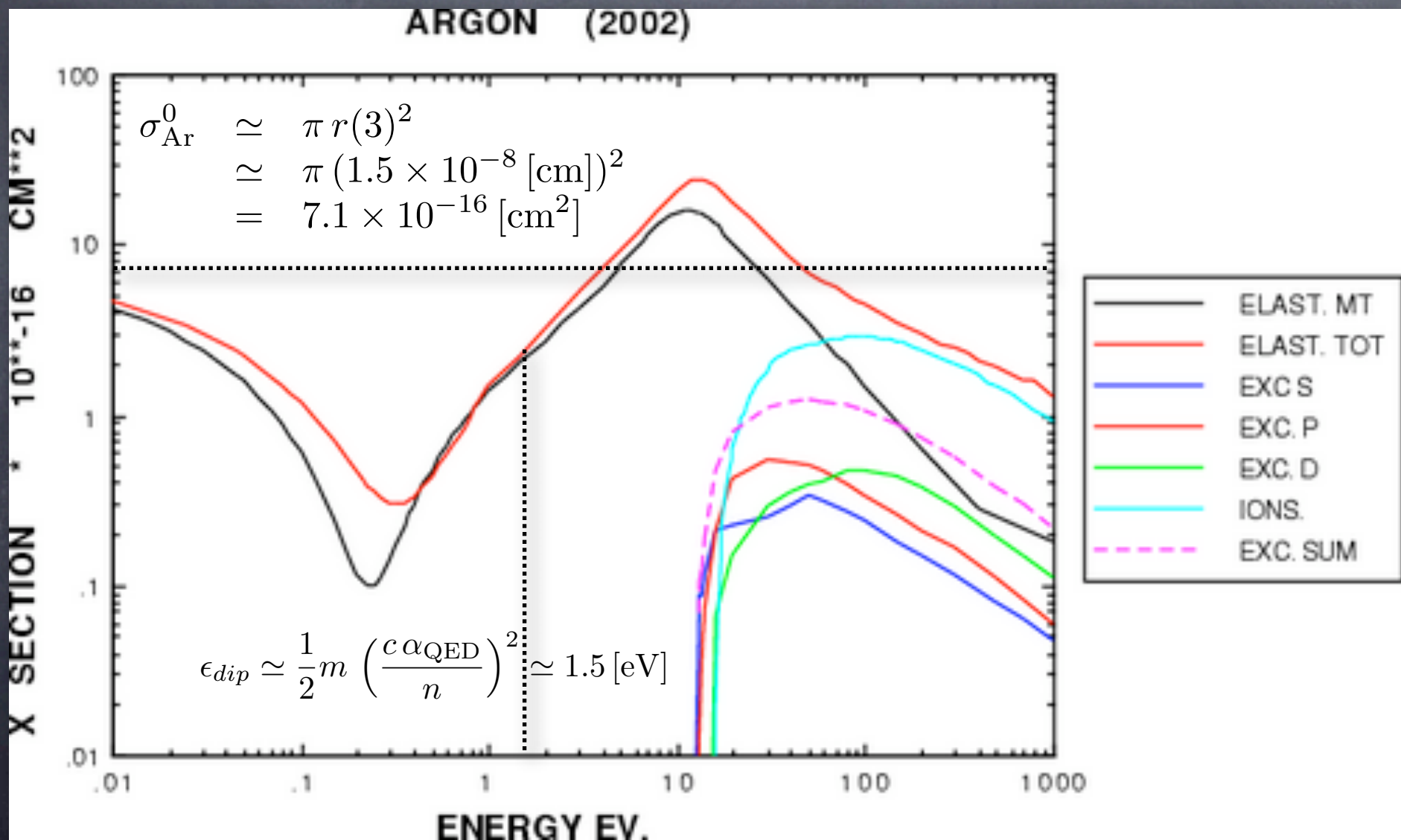
But the life is not so simple, This gives a kind of upper limit, and the real X-section can be much smaller because of the so called Ramsauer effect, a QM effect.

$$\sigma_{\text{Ar}} \propto \left| \sqrt{\sigma_{\text{Ar}}^0} + A \frac{1}{\epsilon - \epsilon_r + i \frac{\Gamma_r}{2}} \right|^2$$

The interference makes a dip below the resonance peak!

Ar Cross Section

That used in Magboltz



Subjects Covered

△ Liberation of electrons by ionization (dE/dx)

○ Classical theory of electron transportation in a chamber gas and its applications

● Behaviors of electrons in E and B fields

● Transport coefficients: V_d , C_d

● Gas amplification

Paul

● Creation of signals

Yulan Li

⊗ Coordinate measurement

Subjects Left Out

- Electron attachment

- CF₄, O₂ contamination, etc. Paul

- Transportation of ions

- +ve ion feed back

Yulan Li

- Ion exchange and aging

These are very important in practice, but simply beyond the scope of my lectures.