



Tracking Detectors

Keisuke Fujii, KEK

Introduction

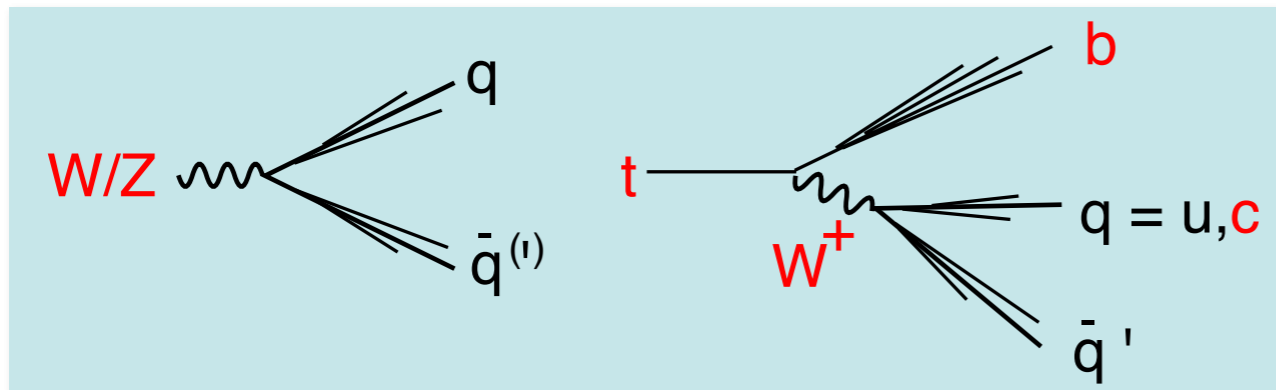
ILC Detectors

CEPC detector should be similar

ILC Experiments

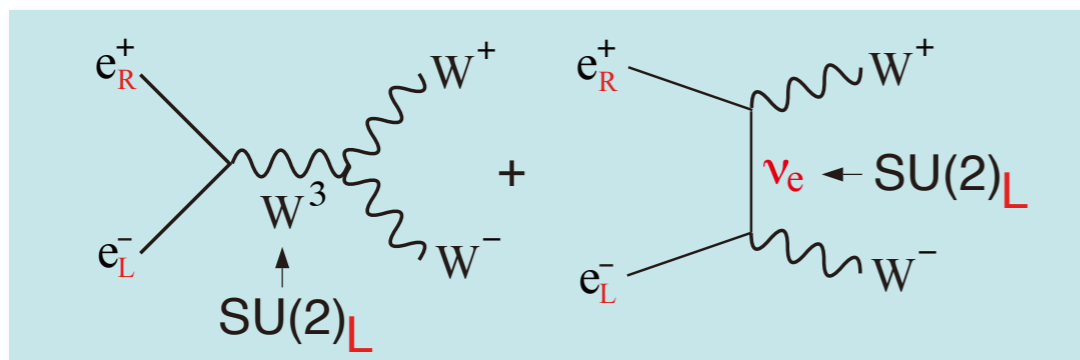
View events as viewing Feynman diagrams

Reconstruct events in terms of (q, l, gb, hb)



Jet invariant mass \rightarrow W/Z/t/h ID \rightarrow p^μ
 \rightarrow angular analysis \rightarrow s^μ
 Missing momentum \rightarrow neutrinos

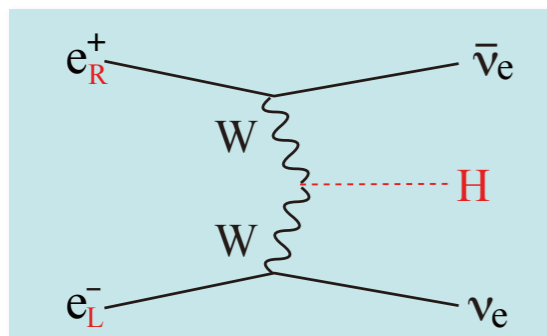
Select Feynman diagrams with polarized beams



To these processes, only left-handed electrons and right-handed positrons contribute !

If you have a wrong combination, cross section is zero.

Beam polarization plays an essential role !



	ILC	CLIC	TLEP/CEPC
Pol (e)	-0.8	-0.8	0
Pol (e)	+0.3	0	0
(σ/σ)	$1.8 \times 1.3 = 2.34$	$1.8 \times 1.0 = 1.8$	1

Beam polarization acts as luminosity doubler !

b/c ID with 2ndary/3tiary vertices

Thin and high resolution vertexing

Particle Flow Analysis

High resolution tracking

high granularity calorimetry

Hermeticity

down to O(10mrad) or better

both ECAL and HCAL inside the solenoid

Detailed **B**aseline Design (TDR vol.4)

arXiv: 1306.6329

- **Large R** with **TPC tracker**
- 32 countries, 151 institutions, ~700 members
- Most members from Asia and Europe
- **B=3.5T**, TPC + Si trackers
- ECal: **R=1.8m**

ILD

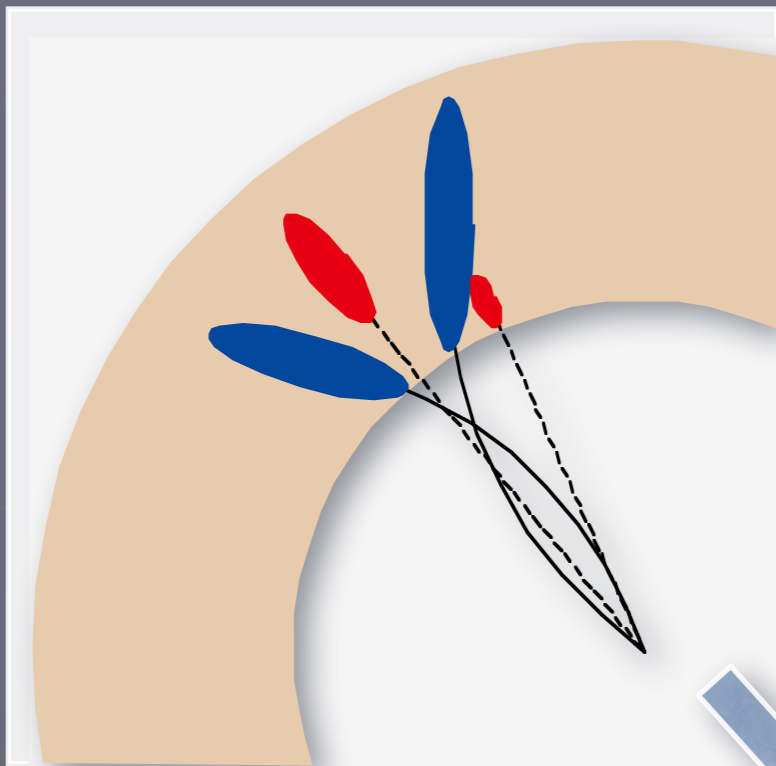
SiD

- **High B** with **Si strip tracker**
- 18 countries, 77 institutions, ~240 members
- Mostly American
- **B=5T**, Si only tracker
- ECal: **R=1.27m**

Both detector concepts are optimized for **Particle
Flow Analysis**

Particle Flow Analysis

How to measure jet energies precisely?



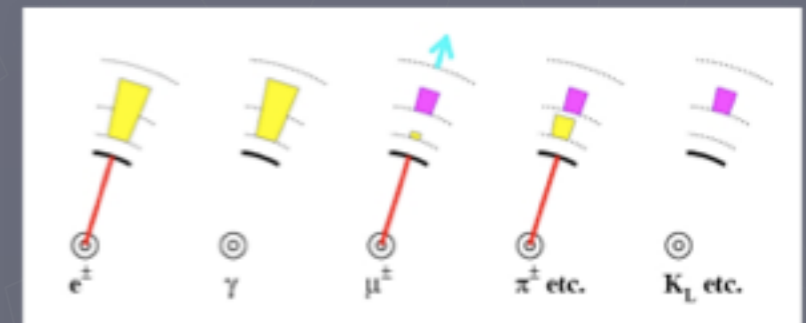
Charged Particles

Tracker's resolution is much better than that of calorimeters

Use tracking devices

Neutral Particles

Use calorimetry

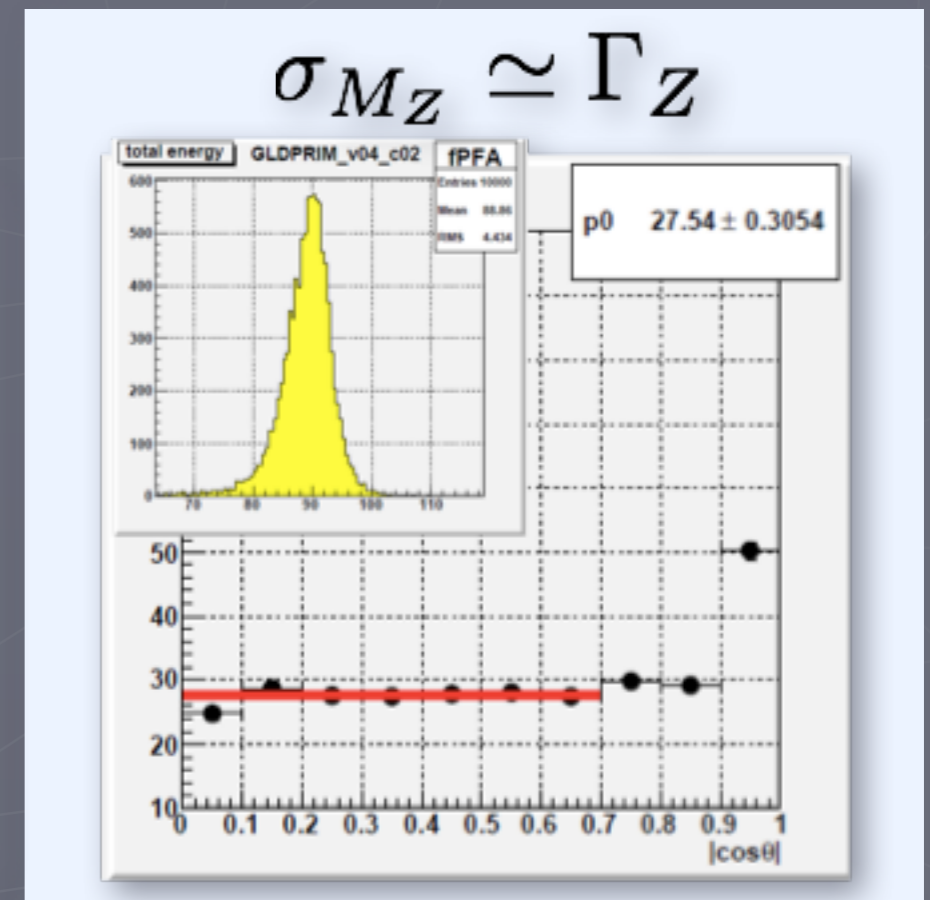
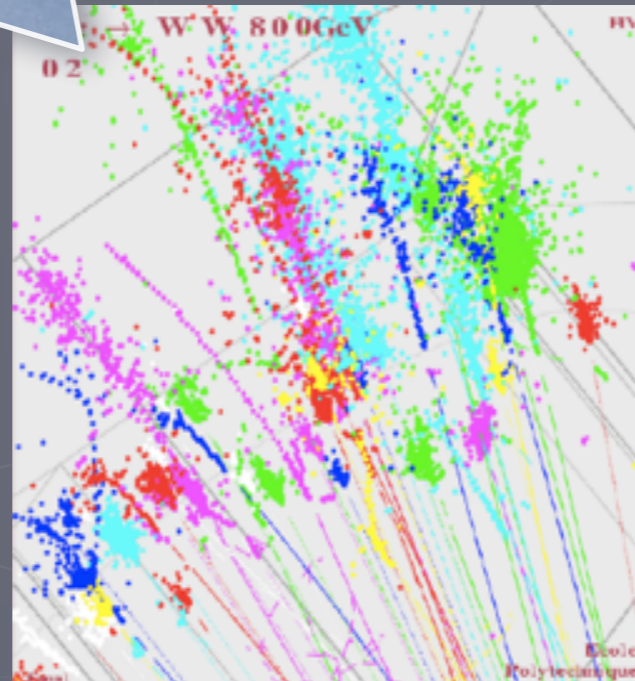


PFA

Remove charged particle signals in calorimeters

Needs 1-to-1 matching of tracks and calorimeter clusters

Needs ultra-high granularity calorimeter



Tracking Detectors

What we want to know

Two 4-vectors:

$$p^\mu = (\mathbf{E}/c, \mathbf{p})$$

$$x^\mu = (ct, \mathbf{x})$$

for every particle produced

Primary purpose of tracking

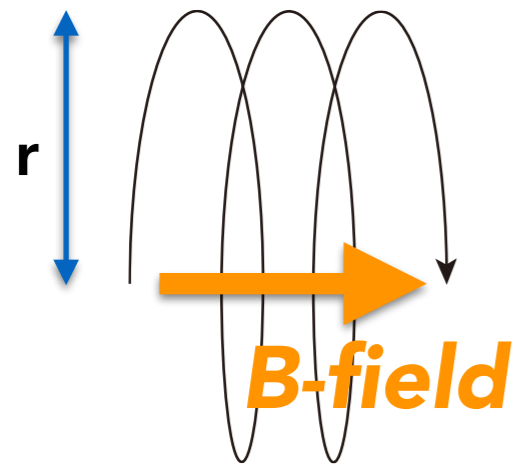
= to measure \mathbf{p} for charged particles



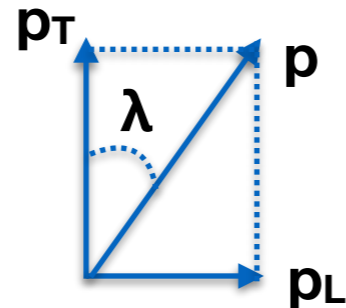
Momentum Measurements



Helical Track



A charged particle follows a helix in uniform magnetic field

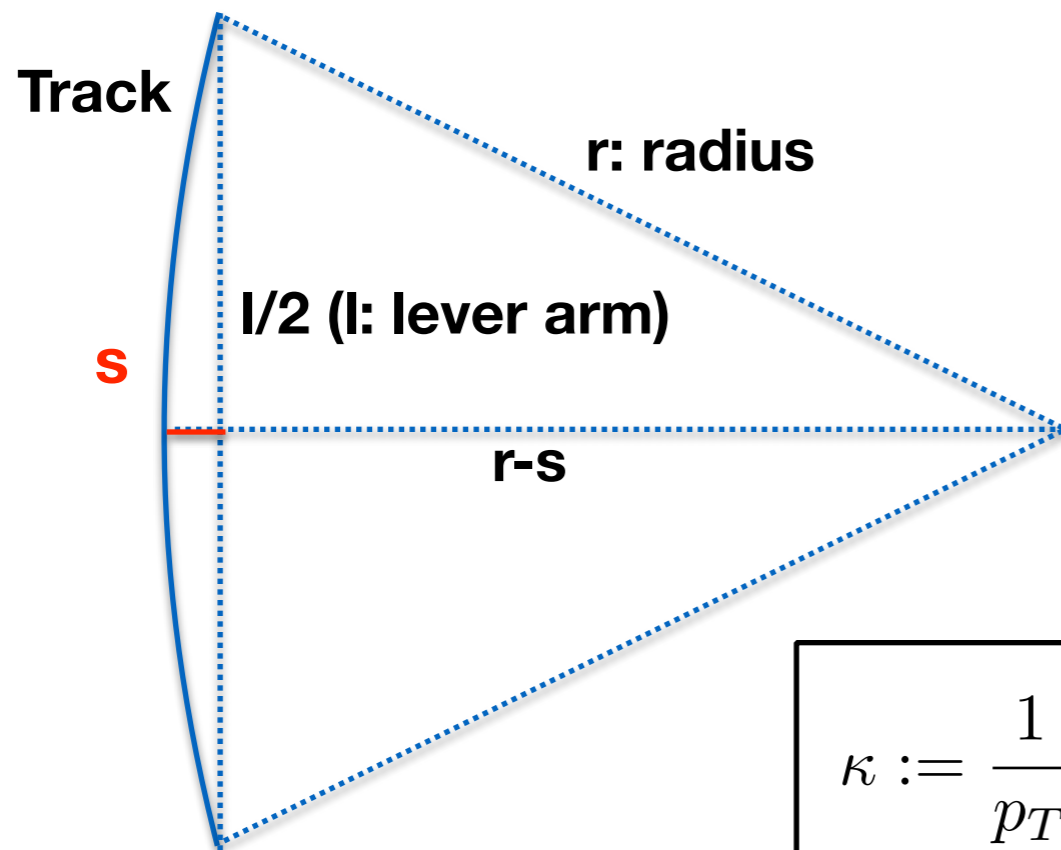


Radius: r → Transverse Momentum: p_T

$$p_T = (1/\alpha)Br$$

$$p_T [\text{GeV}/c] = 0.3 \cdot B[\text{T}] \cdot r[\text{m}]$$

Radius from sagitta



Dip angle: λ → Longitudinal Momentum: p_L

$$p_L = p_T \tan \lambda$$

Sagitta: s

$$r^2 = (l/2)^2 + (r - s)^2 \quad (s \ll l)$$

$$\longrightarrow 2rs = (l/2)^2 + s^2 \simeq l^2/4$$

$$\longrightarrow r \simeq l^2/(8s)$$

$$\kappa := \frac{1}{p_T} \simeq \left(\frac{8\alpha}{Bl^2} \right) s \longrightarrow \sigma_{\kappa}^{meas} := \frac{\sigma_{p_T}}{p_T^2} \simeq \left(\frac{8\alpha}{Bl^2} \right) \sigma_s$$



Gluckstern Formula



Transverse momentum: p_T $\kappa := 1/p_T$

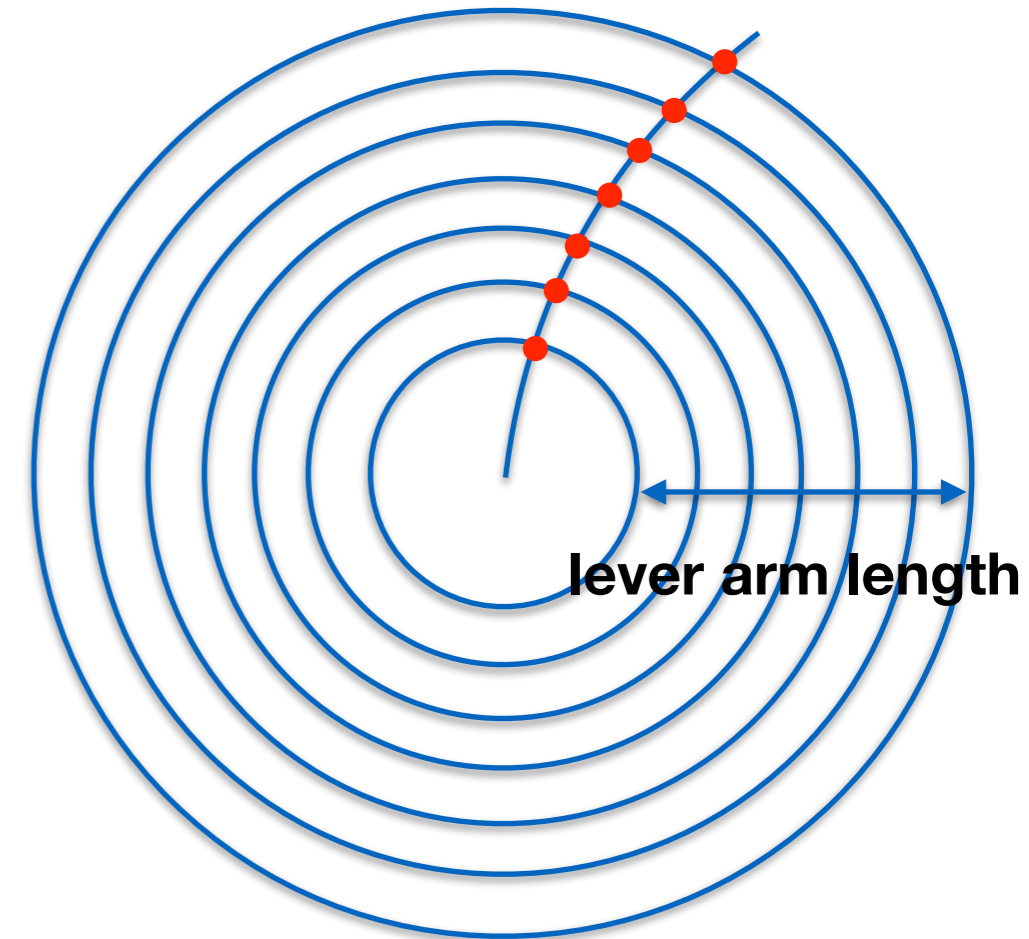
$$\sigma_{\kappa}^2 = (\sigma_{\kappa}^{meas})^2 + (\sigma_{\kappa}^{MS})^2$$

Detector
resolution

Multiple
scattering

$$\sigma_{\kappa}^{meas} \simeq \left(\frac{\alpha \sigma_x}{Bl^2} \right) \sqrt{\frac{720}{n+4}}$$

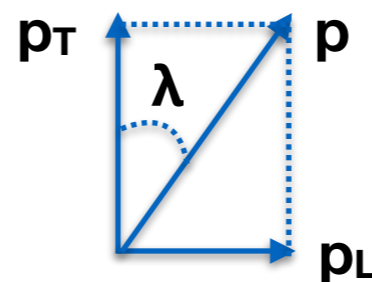
$$\sigma_{\kappa}^{MS} \simeq \left(\frac{\alpha C}{Bl} \right) \sqrt{\frac{10}{7} \left(\frac{X}{X_0} \right)} \cdot \kappa$$



n equally spaced sampling points for tracking

Total momentum:

$$p = p_t \sqrt{1 + \tan^2 \lambda}$$



Dip angle: λ

$$\sigma_{\tan \lambda} \simeq \sqrt{\left(\frac{\sigma_z}{l} \right)^2 \left(\frac{12}{n} \right) + (1 + \tan^2 \lambda) \left(\frac{C}{p_T} \right)^2 \left(\frac{13}{35} \left(\frac{X}{X_0} \right) \right)}$$

- $\sigma_x =$ spatial resolution in the $r-\phi$ plane per point
- $n =$ the number of sampling points
- $\alpha =$ 333.56 (cm · T · GeV⁻¹)
- $C =$ 0.0141 (GeV)
- $(X/X_0) =$ thickness measured in radiation length units
- $l =$ lever arm length (cm)
- $B =$ magnetic field (T)



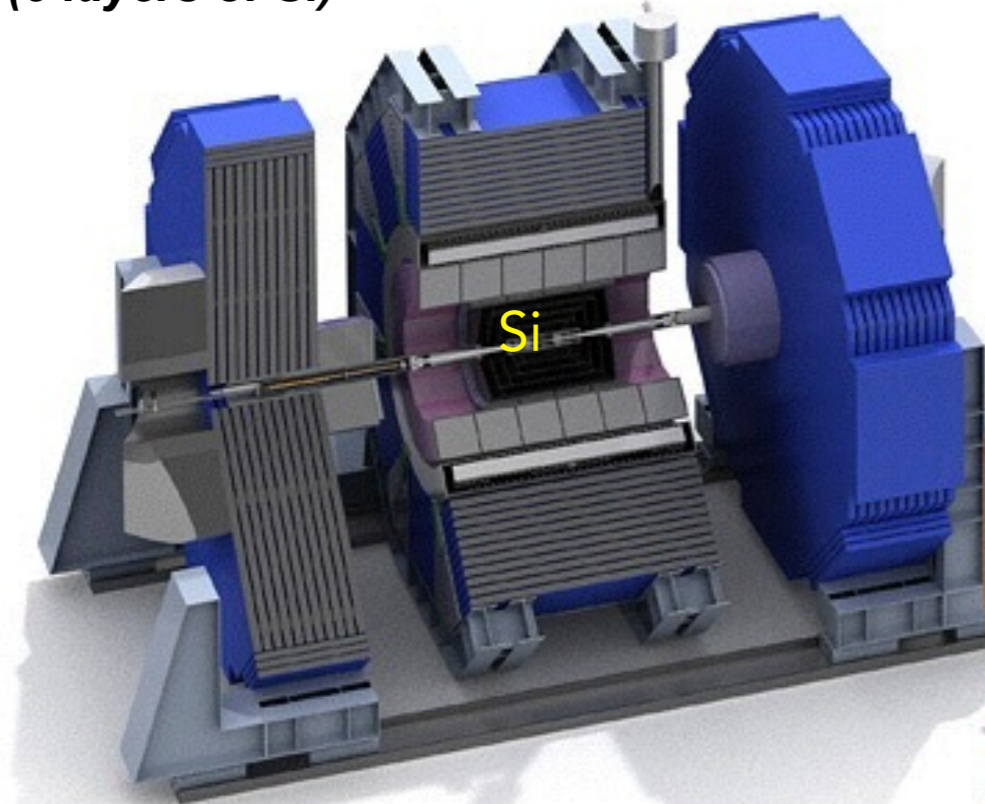
Two Options



SiD

*High B, excellent σ_x
but small n*

*Reasonably low material budget
(5 layers of Si)*



$$\sigma_{\kappa}^2 = (\sigma_{\kappa}^{meas})^2 + (\sigma_{\kappa}^{MS})^2$$

$$\sigma_{\kappa}^{meas} \simeq \left(\frac{\alpha \sigma_x}{Bl^2} \right) \sqrt{\frac{720}{n+4}}$$

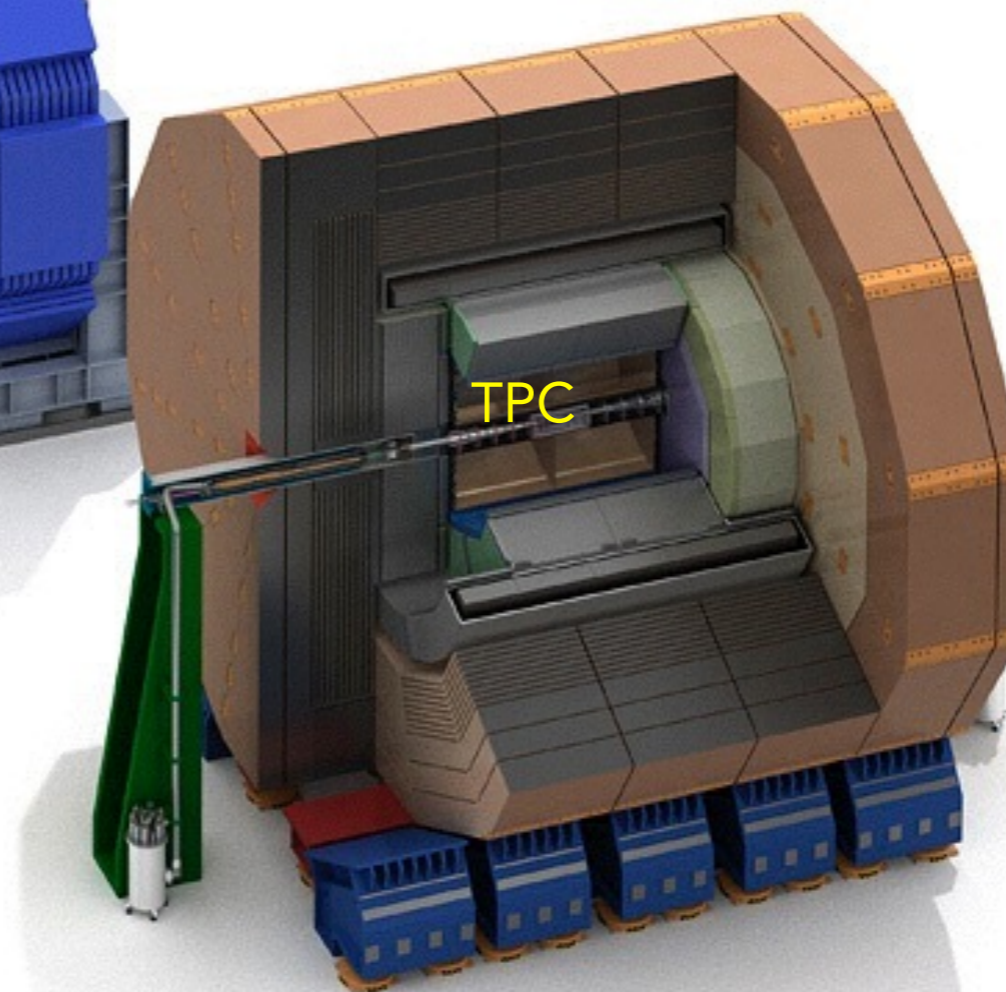
$$\sigma_{\kappa}^{MS} \simeq \left(\frac{\alpha C}{Bl} \right) \sqrt{\frac{10}{7} \left(\frac{X}{X_0} \right)} \cdot \kappa$$

ILD

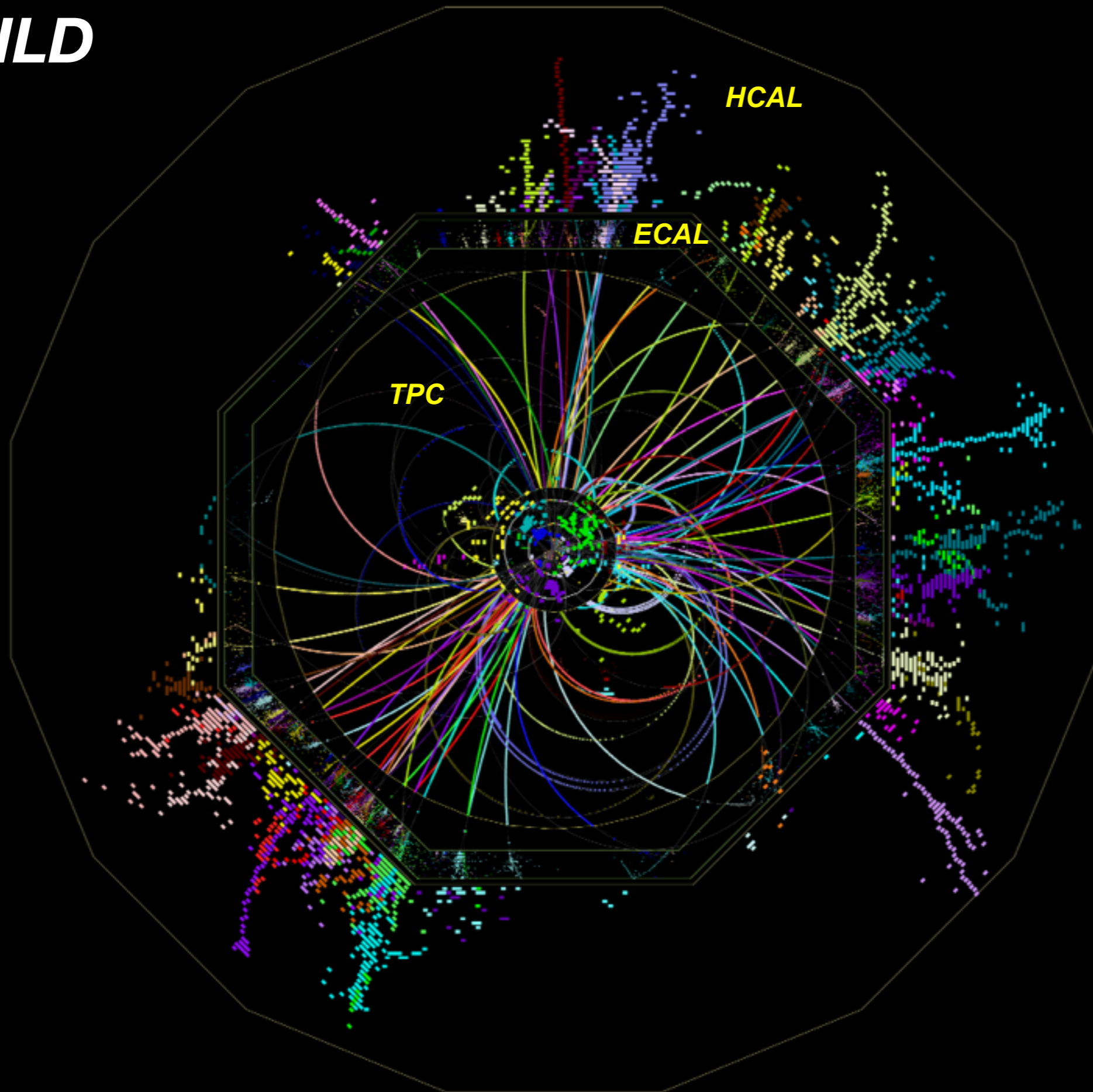
*Large l,
large n
but moderate σ_x*

*Low material
budget (gas)*

Pictorial tracking



ILD



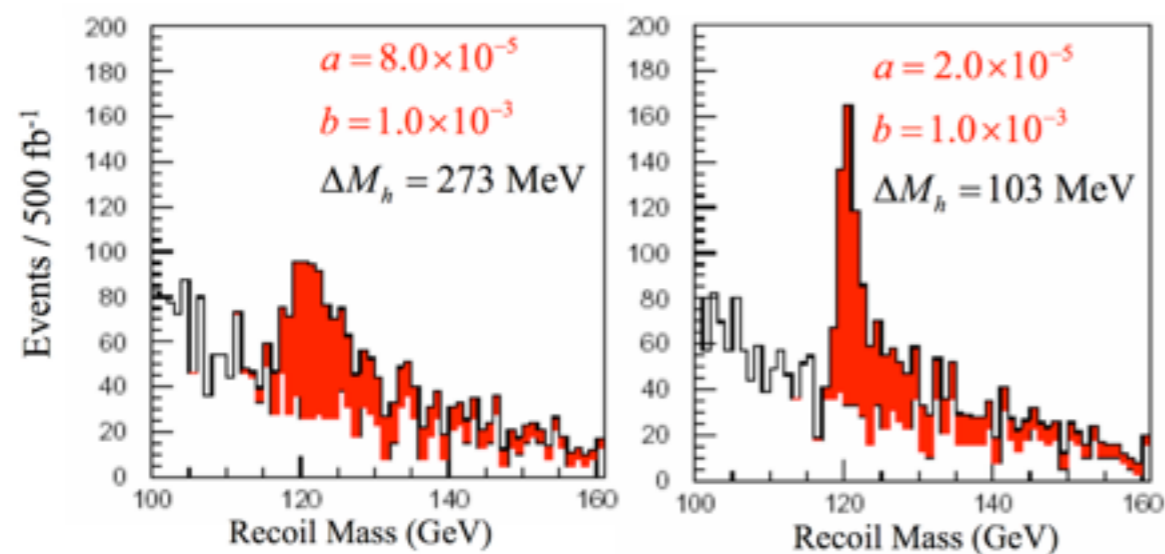
tth @ 500 GeV



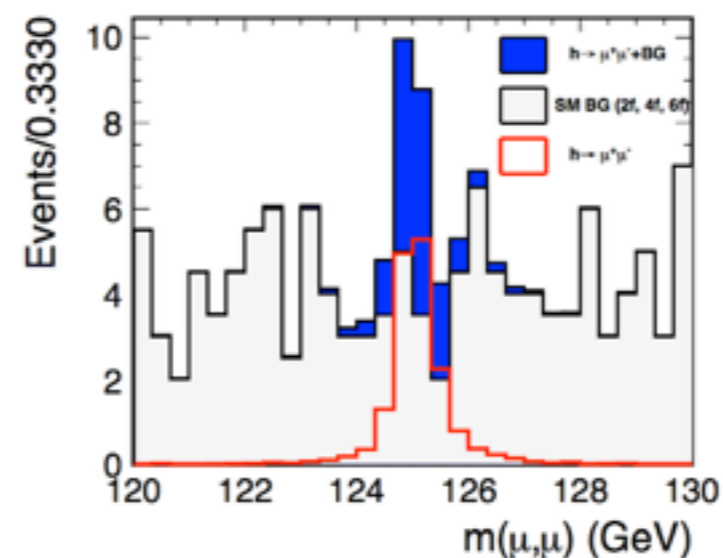
Performance Goals



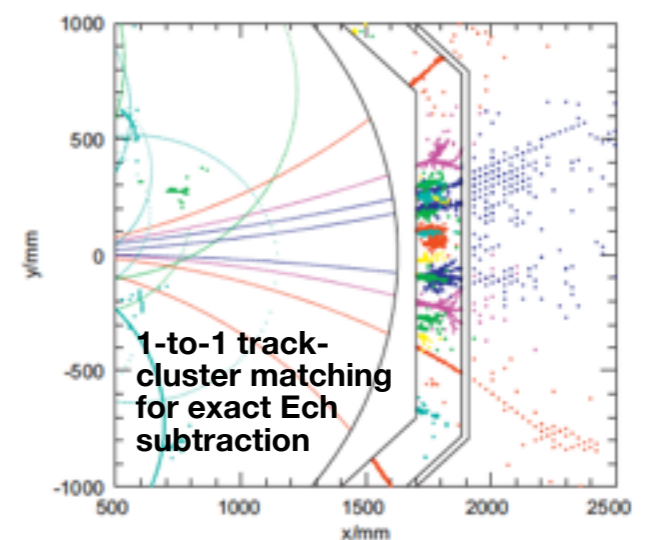
- Momentum Resolution:** $\sigma(1/p_t) = 2 \times 10^{-5} \text{ (GeV}^{-1}\text{)}$
>200 sampling points along a track with a spatial resolution better than $\sigma_{r\phi} \sim 100 \text{ }\mu\text{m}$ over the full drift length of >2m in B=3.5T (recoil mass, $H \rightarrow \mu^+\mu^-$).
- High Efficiency:** 2-track separation better than $\sim 2\text{mm}$ to assure essentially 100% tracking efficiency for PFA in jetty events.
High tracking efficiency also requires **minimization of dead spaces** near the boundaries of readout modules.
- Minimum material:** for PFA calorimeters behind, also to facilitate extrapolation to the inner Si tracker and the vertex detector



Recoil Mass Measurement

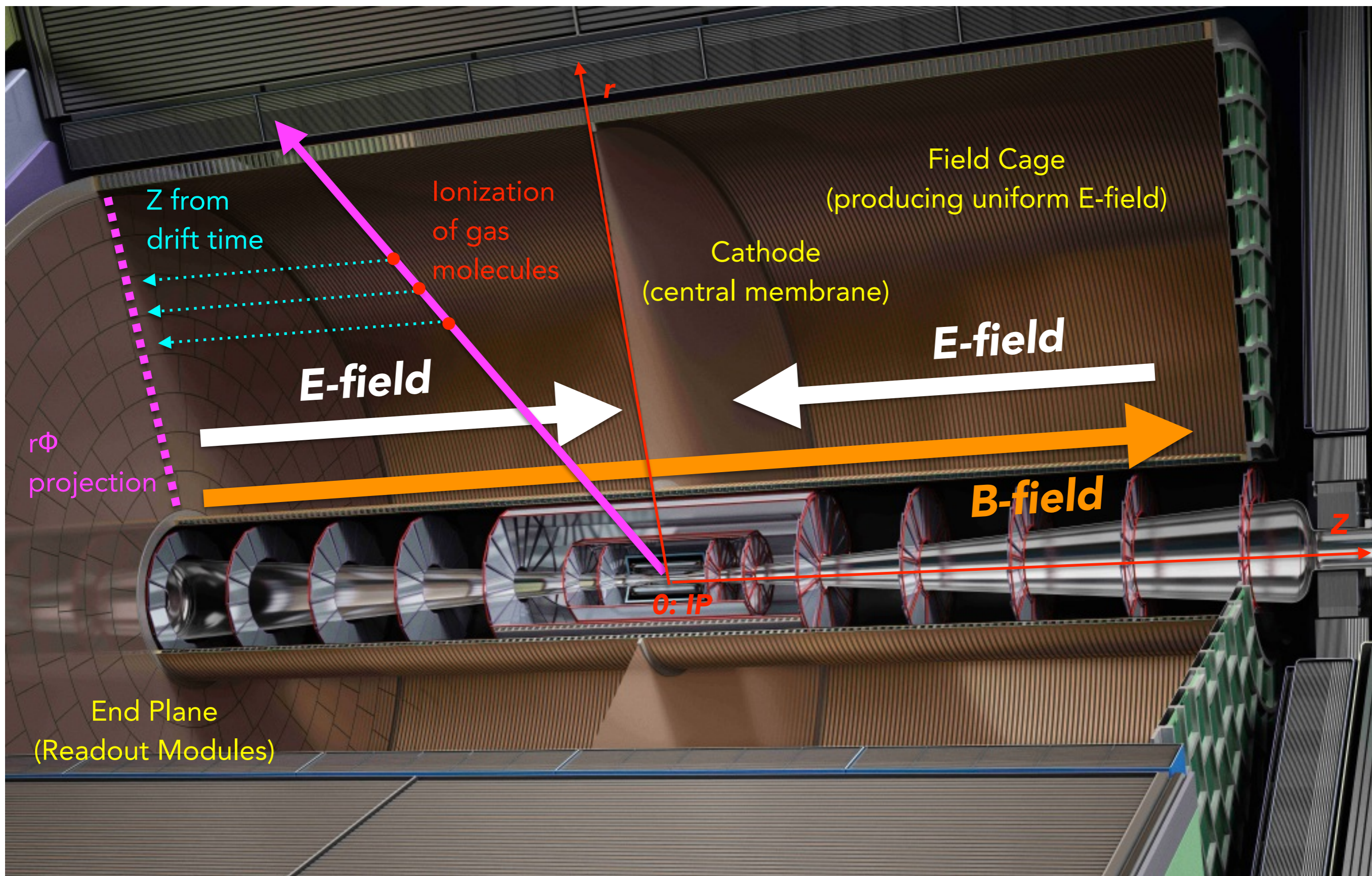


$H \rightarrow \mu^+\mu^-$



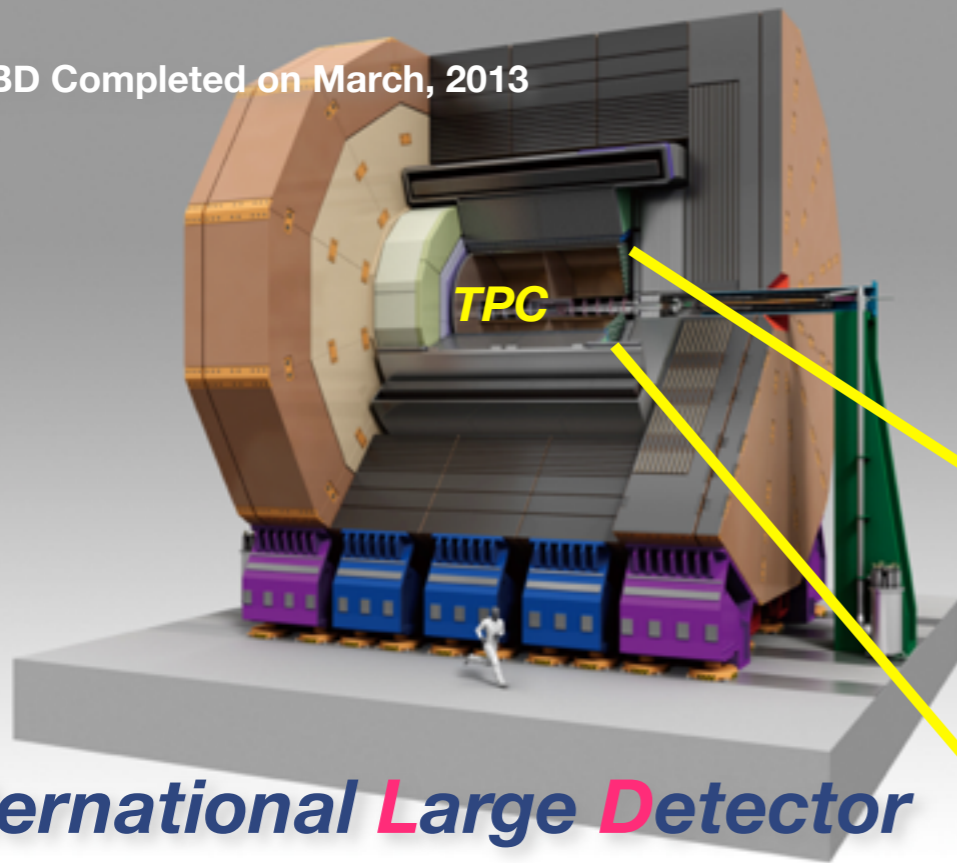
Particle Flow Analysis

What is **T**ime **P**rojection **C**hamber?



LC-TPC

ILD DBD Completed on March, 2013

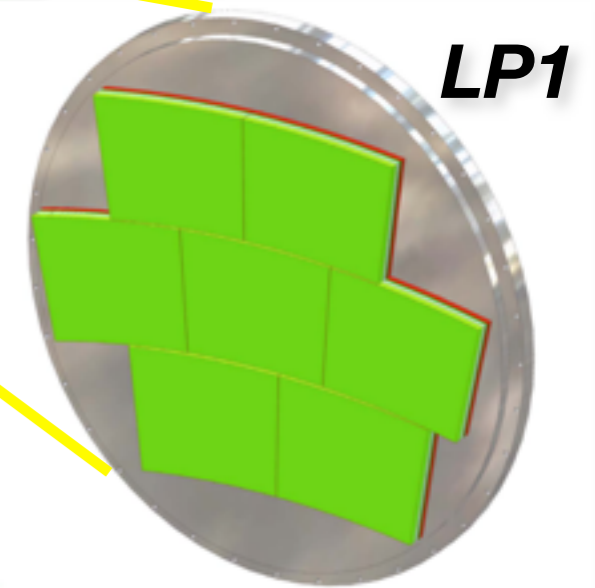
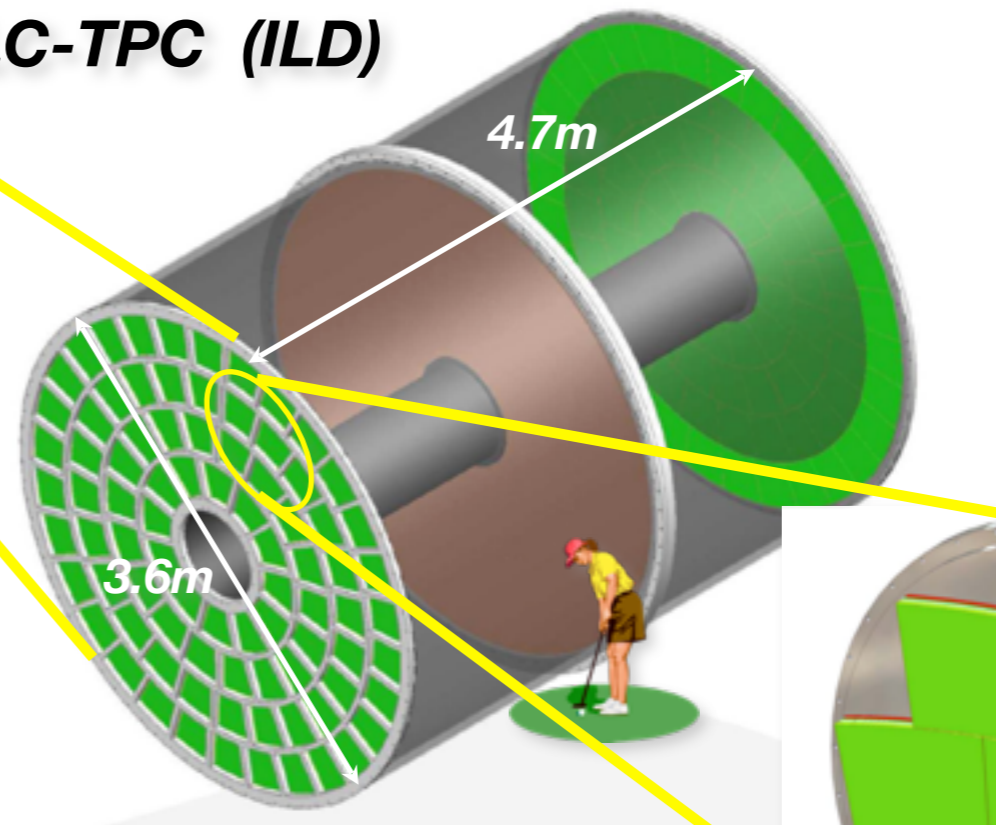


International Large Detector

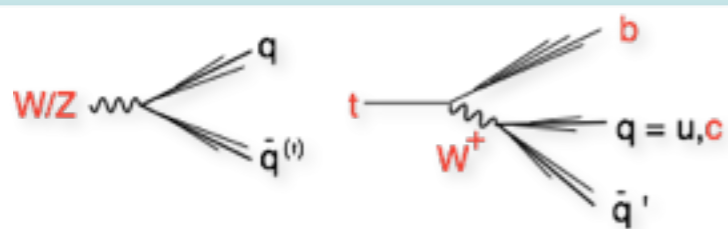
Performance Goals as compared to LHC detectors

Vertex resolution	2-7 times better
Momentum resolution	10 times better
Jet energy resolution	2 times better

LC-TPC (ILD)



ILD : optimized for Particle Flow Analysis



Highly efficient tracking in a jetty environment is an essential ingredient for PFA

Micro Pattern Gas Detector readout TPC provides pictorial 3D tracking by ~200 space points with $\sigma_{r\phi} \sim 100 \mu\text{m}$ and two-hit separation of ~2mm

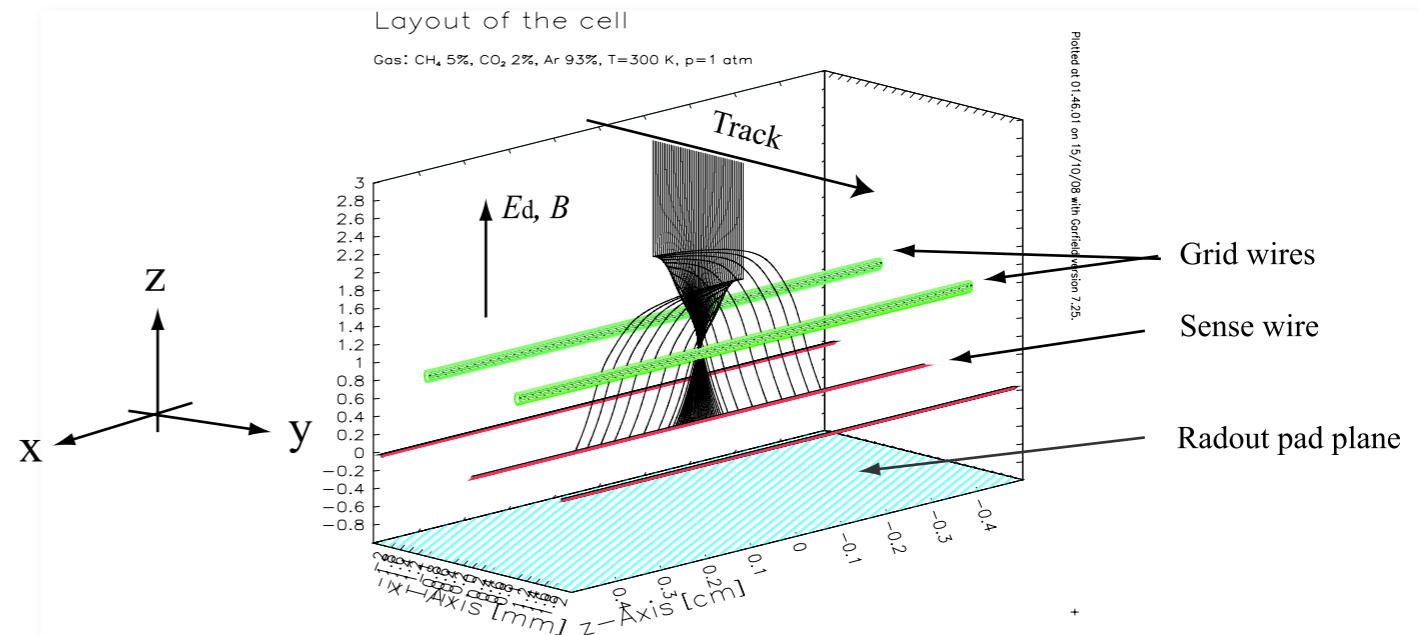
Large Prototype being tested at DESY



Why MPGD Readout?



- We need high (>3 T) B field to confine e⁺e⁻ pair BG from beam-beam interactions, then **ExB is too big** for conventional **MWPC** readout
- 2mm 2-track separation is difficult with MWPC readout
- Thick frames are unavoidable for MWPC readout

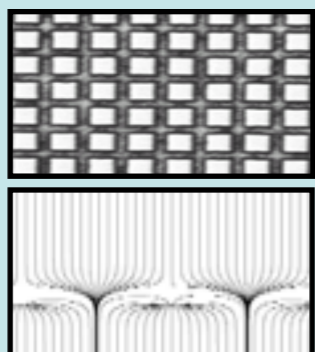


ExB spreads seed electrons along the sense wires, then avalanche fluctuation limits the spatial resolution!

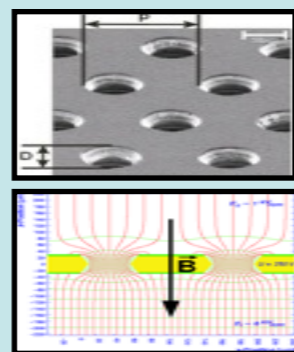


Micro-Pattern Gas Detectors

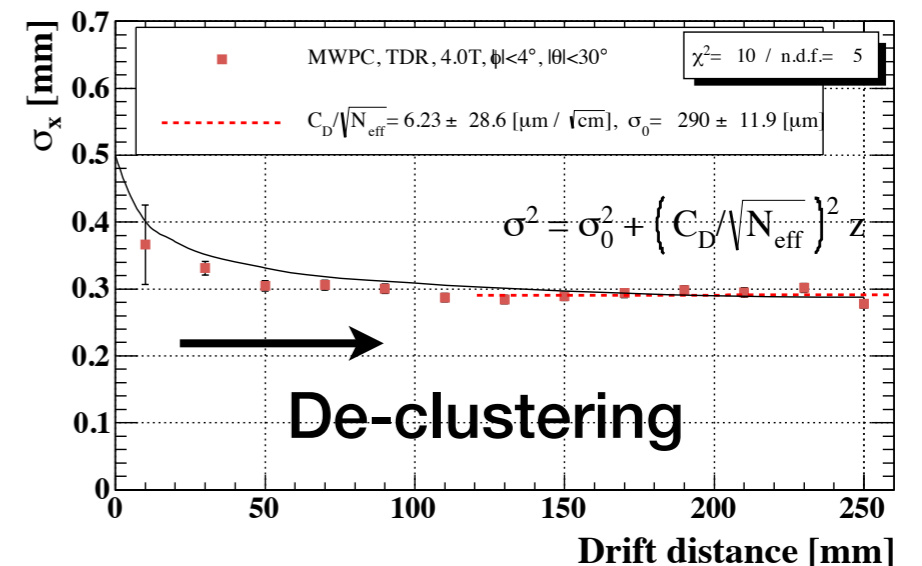
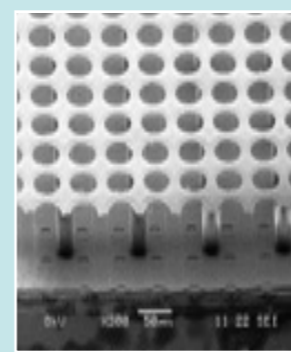
Micromegas



GEM



InGrid TimePix



Pre-LCTPC group incl. the FJ teams excluded MWPC together with a small prototype TPC!



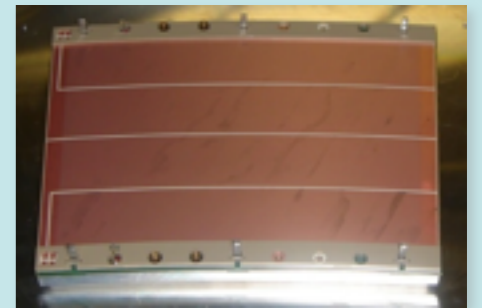
MPGD Options



After the initial stage of R&D with many small TPC prototypes, we are left with three options of MPGD TPC readout technologies for ILC, being tested at the Large prototype (LP) TPC at DESY.

I. Analog (Pad) TPC: Subject to the gas gain fluctuation in the gas amplification. Need to spread the avalanche charge for charge centroid.

Asian GEM module



(1) Multi layer GEM with the standard pad ($\sim 1 \times 5 \text{mm}^2$) readout :
(charge spread by diffusion)

Asian (KEK-Saga-Tsinghua) Module, DESY module

(2) Micromegas with the resistive-anode (pad: $\sim 3 \times 7 \text{mm}^2$) readout :
Saclay-Carleton Module

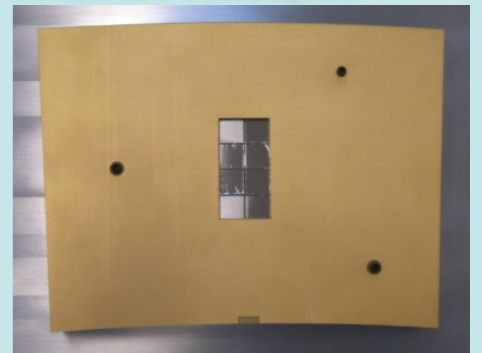
MM (resistive anode)



II. Digital (Pixel) TPC: Free from the gas gain fluctuation. Expect 20-30% improvement of position resolution in the case of digital readout.
No angular pad effect.

Theoretically the best but not yet ready for full implementation of a module.

InGrid+Timepix



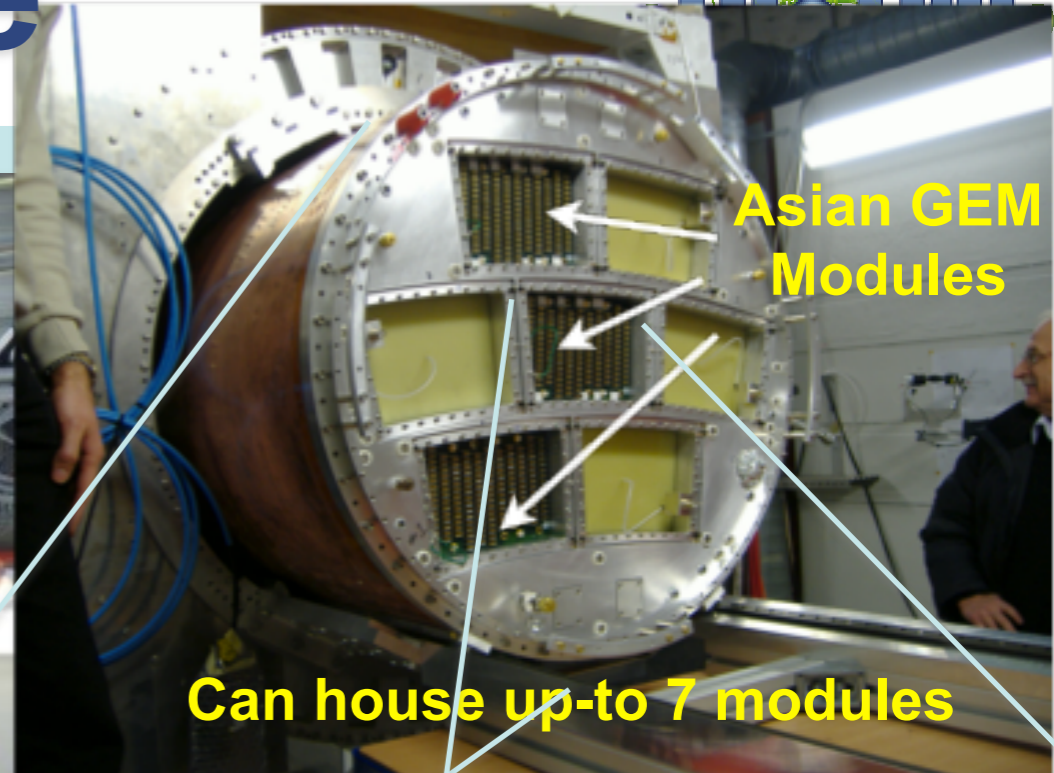
(3) InGrid Micromegas mesh on Timepix chips (pixel: $\sim 50 \times 50 \mu\text{m}^2$)
NIKHEF-Saclay Module, Bonn-module



Large Prototype



GM cryo-coolers

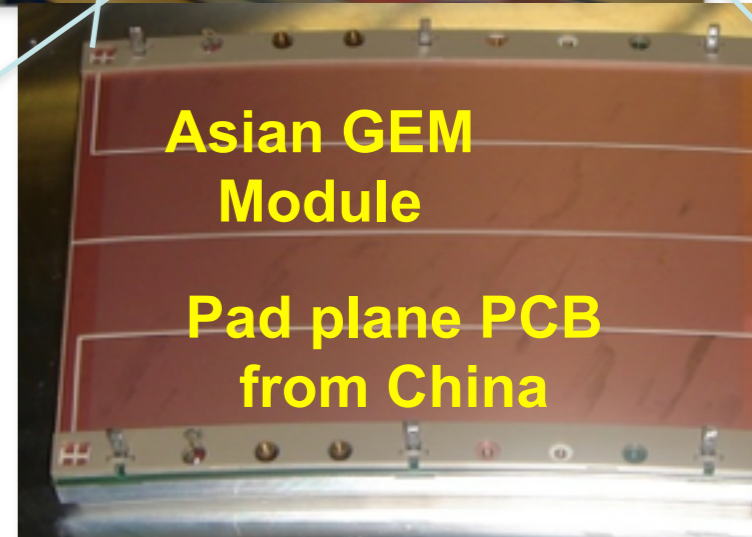


Asian GEM Modules

Can house up-to 7 modules

PCMAG from KEK modified by Toshiba under the framework of DESY-KEK collaboration in JFY2011 to allow Liq.He-less operation

Being used for test beam experiments since June 2012



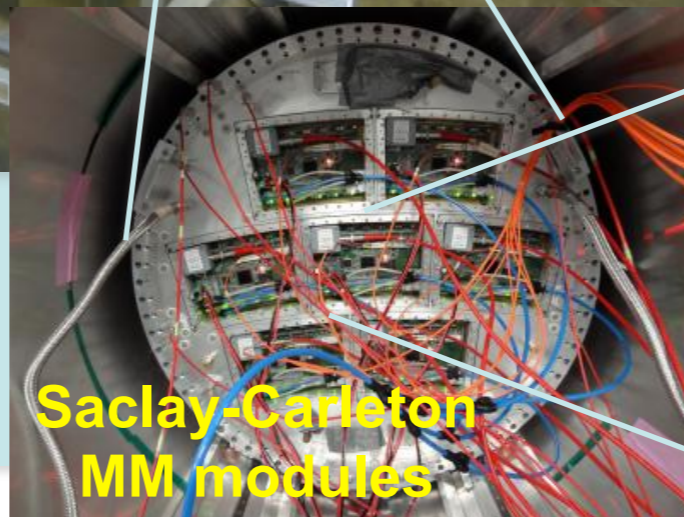
Asian GEM Module

Pad plane PCB from China

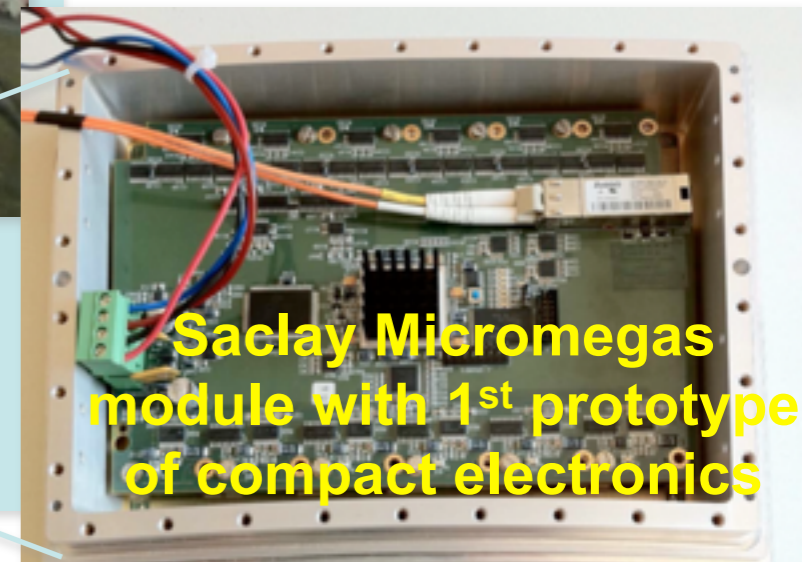


5GeV electron beam

Large Prototype test beam



Saclay-Carleton MM modules



Saclay Micromegas module with 1st prototype of compact electronics

Basic Operational Principle of MPGD Readout TPC

Basic Physics Behind Operation of TPC

Part I

-- Fundamental Processes in the TPC --

Keisuke Fujii

iSTEP 2014, IHEP Beijing, Aug. 2014

Purpose

I will focus on very basic principles, trying to prepare you, students, for more advanced topics containing more practical and technical aspects.

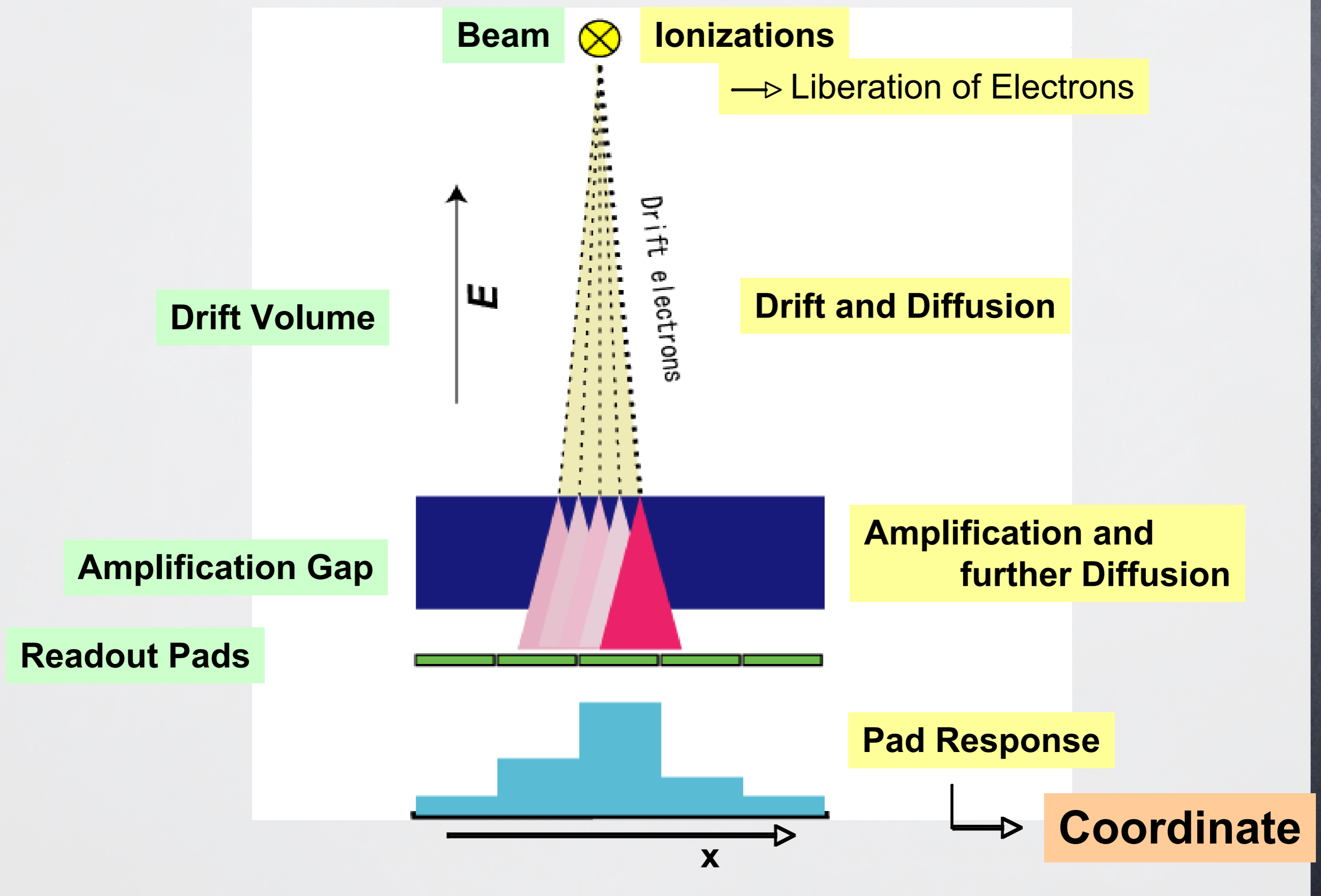
Emphasis will be put on concepts and philosophy, and hence practical examples will be minimum, for them take a look at excellent text books such as

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

F.Sauli 1977: CERN 77-09

W.Blum & L.Rolandi 1993, 2008

Fundamental Processes



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
- Positive ion effects

Liberation of Electrons

Through Ionization of Gas Molecules
By a Fast Moving Charged Particle

This part will be brief, though it is a deep subject.

Ionizing Collisions

Various Ionization Mechanisms

Primary Direct Ionization

A charged particle going through a chamber gas ionizes gas molecules along its path and leaves a track of ionization. This is called primary ionization. The ionizing collisions are statistically independent, and hence the number of such collisions obeys the Poisson distribution:

$$P(n; \bar{n}) = \frac{\bar{n}^n}{n!} e^{-\bar{n}}$$

where the average number of collisions is given by the thickness (L) of the medium and the mean free path (λ) as

$$\bar{n} = L/\lambda$$

The mean free path is of course related to the cross section per electron in the gas and the electron density in the gas.

$$N\sigma_I \lambda = 1$$

The probability distribution for the free flight path (l) is then given by

$$f(l; \lambda) dl = P(0; l/\lambda) P(1; dl/\lambda) = e^{-l/\lambda} \frac{dl}{\lambda}$$

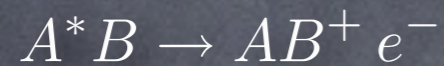
The average number of ionizing collisions per 1cm is about 28 for a minimum ionizing particle passing through an Ar gas at 1atm. This corresponds to an ionization cross section of

$$\sigma_I(\text{Ar}) \simeq 10^{-18} [\text{cm}^2] \sim \pi R_{\text{Ar}}^2 \times Z_{\text{Ar}} \alpha_{\text{QED}}^2$$

Secondary Ionization

The electrons kicked out from molecules, if energetic enough, will further ionize gas molecules. Some of the gas molecules might be excited to some intermediate state that can lead to further ionizations through a

process like



where A^* is an excited molecule and B is a molecule with an ionization potential that is lower than the excitation energy of A^* .

A^* is often a metastable excited state of a noble gas used as the main gas component (e.g. Ar) and B is often a quencher added to stabilize the gas amplification process.

A^* can also be an optical excitation with a long life time.

A^* = metastable \rightarrow Penning Effect

A^* = optical excitation \rightarrow Jesse Effect

Average Energy for Ionization

Only a certain fraction of the energy loss by the fast charged particle is used for ionization. We define "W" as the average energy required for the creation of a single ionization electron. Then the average number of ionization electrons along a track

of a length "L" is given by

$$\langle n_I \rangle = \left\langle \frac{dE}{dx} \right\rangle \frac{L}{W}$$

The "W" depends on the gas and the nature of the incident particle, but it is known to be independent of incident energy if $E >$ a few keV for electrons or if $E >$ a few MeV for alpha-particles.

For a noble gas, "W" ranges from 46 eV for He to 22 eV for Xe. For Ar it is 26 eV.

The "W" values are typically a factor of 1.5 to 2 larger than the ionization potentials.

In order to see how the average energy loss depends on the particle's speed or on the nature of the gas, and to understand the distribution around the average, let us review next the Allison-Cobb formulation of the energy loss process.

Allison-Cobb Formulation

dE/dx as a photo-absorption/ionization by a virtual photon

A Charged Particle in a Dielectric

The energy loss of a charged particle that passes through a dielectric medium is due to the negative work done by the E-field created by the electrons and the nuclei of the molecules making up the medium:

$$dE/dx \cdot dx = -e \left(\sum_a \mathbf{E}_a \right) \cdot dx$$

where e is the particle charge and the sum is over all the charges in the medium.

Averaging the both sides over a small tube around the incident particle, we have

$$\langle dE/dx \rangle \cdot dx = -e \mathbf{E} \cdot dx$$

with

$$\mathbf{E} = \left\langle \sum_a \mathbf{E}_a \right\rangle$$

If we can determine the E-field by solving the Maxwell equations, we can get dE/dx

$$\langle dE/dx \rangle = -e \mathbf{E}(c\beta t, t) \cdot \beta / \beta$$

The Maxwell equations

The Maxwell equations in a dielectric with a magnetic permeability of one ($B = H$) read

$$\nabla \cdot \mathbf{B} = 0$$

$$\nabla \times \mathbf{E} = -\frac{1}{c} \frac{\partial}{\partial t} \mathbf{B}$$

$$\nabla \cdot \mathbf{D} = 4\pi\rho$$

$$\nabla \times \mathbf{B} = \frac{1}{c} \frac{\partial}{\partial t} \mathbf{D} + \frac{4\pi}{c} \mathbf{j}$$

The charge and current densities are

$$\rho(\mathbf{x}, t) = e \delta^3(\mathbf{x} - c\beta t)$$

$$\mathbf{j}(\mathbf{x}, t) = c\beta \rho(\mathbf{x}, t)$$

where $c\beta$ is the velocity of the charged particle that can be regarded as constant during its passage through the dielectric medium.

In order to close the Maxwell equations we need a material equation for the dielectric medium:

$$\mathbf{D}(\mathbf{x}, t) = \mathbf{E}(\mathbf{x}, t) + \int_0^\infty d\tau \int_{|\boldsymbol{\xi}| < c\beta\tau} d^3\xi G(|\boldsymbol{\xi}|, \tau) \mathbf{E}(\mathbf{x} - \boldsymbol{\xi}, t - \tau)$$

which expresses the dependence of the electric flux density on the electric fields at causally connected space-time points through a Green function G .

Defining Fourier transform of f as

$$\tilde{f}(\mathbf{k}, \omega) \equiv \int \frac{d^3\mathbf{x} dt}{(2\pi)^2} f(\mathbf{x}, t) e^{-i(\mathbf{k}\cdot\mathbf{x} - \omega t)}$$

we have

$$\tilde{\mathbf{D}}(\mathbf{k}, \omega) = \epsilon(k, \omega) \tilde{\mathbf{E}}(\mathbf{k}, \omega)$$

with

$$\epsilon(k, \omega) = 1 + \int_0^\infty d\tau \int_{|\boldsymbol{\xi}| < c\beta\tau} d^3\xi G(|\boldsymbol{\xi}|, \tau) e^{i(\mathbf{k}\cdot\boldsymbol{\xi} - \omega\tau)}$$

The dielectric constant being independent of the direction of the wave vector shows the isotropy of the dielectric medium. Notice that the \mathbf{E} - and \mathbf{D} -fields being real implies

$$\epsilon^*(k, \omega^*) = \epsilon(k, -\omega)$$

In the limit of $\omega \rightarrow \infty$ we have

$$\epsilon(k, \omega) - 1 \simeq \frac{i\tilde{G}(0)}{\omega} - \frac{\tilde{G}'(0)}{\omega^2} + \dots = -\frac{\tilde{G}'(0)}{\omega^2} + \dots$$

with

$$\int_{|\boldsymbol{\xi}| < c\beta\tau} d^3\xi G(|\boldsymbol{\xi}|, \tau) e^{i\mathbf{k}\cdot\boldsymbol{\xi}} \simeq \int_{|\boldsymbol{\xi}| < c\beta\tau} d^3\xi G(|\boldsymbol{\xi}|, \tau) = \tilde{G}(\tau)$$

since only the region near $\tau \simeq 0$ contributes.

The Solution

With the scalar and vector potentials

$$\tilde{\mathbf{B}}(\mathbf{k}, \omega) = i\mathbf{k} \times \tilde{\mathbf{A}}(\mathbf{k}, \omega)$$

$$\tilde{\mathbf{E}}(\mathbf{k}, \omega) = \frac{i\omega}{c} \tilde{\mathbf{A}}(\mathbf{k}, \omega) - i\mathbf{k}\tilde{\phi}(\mathbf{k}, \omega)$$

in the Coulomb gauge

$$\tilde{\mathbf{B}}(\mathbf{k}, i\mathbf{k} \cdot \tilde{\mathbf{A}}(\mathbf{k}, \omega) = 0$$

we can translate the Maxwell eqs. into

$$k^2 \epsilon \tilde{\phi}(\mathbf{k}, \omega) = 2e \delta(\omega - c\boldsymbol{\beta} \cdot \mathbf{k})$$

$$k^2 \tilde{\mathbf{A}}(\mathbf{k}, \omega) = \frac{\epsilon\omega^2}{c^2} \tilde{\mathbf{A}}(\mathbf{k}, \omega) - \frac{\epsilon\omega\mathbf{k}}{c} \tilde{\phi}(\mathbf{k}, \omega) + 2e\boldsymbol{\beta} \delta(\omega - c\boldsymbol{\beta} \cdot \mathbf{k})$$

The solution is hence given by

$$\tilde{\phi}(\mathbf{k}, \omega) = \frac{2e}{\epsilon k^2} \delta(\omega - c\boldsymbol{\beta} \cdot \mathbf{k})$$

$$\tilde{\mathbf{A}}(\mathbf{k}, \omega) = 2e \frac{\omega\mathbf{k}/ck^2 - \boldsymbol{\beta}}{\epsilon\omega^2/c^2 - k^2} \delta(\omega - c\boldsymbol{\beta} \cdot \mathbf{k})$$

The Energy Loss Formula

Putting them together into the energy loss formula after inverse Fourier transform, we obtain

$$\begin{aligned} \langle dE/dx \rangle &= -e (\boldsymbol{\beta}/\beta) \cdot \mathbf{E}(c\boldsymbol{\beta}t, t) \\ &= -e \int \frac{d^3\mathbf{k} d\omega}{(2\pi)^2} (\boldsymbol{\beta}/\beta) \cdot \tilde{\mathbf{E}}(\mathbf{k}, \omega) e^{i(\mathbf{k} \cdot c\boldsymbol{\beta}t - \omega t)} \\ &= -\frac{2e^2}{(2\pi)\beta^2 c^2} \int_{-\infty}^{+\infty} d\omega \int_{|\omega|/c\beta}^{\infty} dk i(\omega k) \left[\frac{\omega^2/k^2 c^2 - \beta^2}{\epsilon\omega^2/c^2 - k^2} - \frac{1}{k^2 \epsilon} \right] \end{aligned}$$

or with $\epsilon^*(k, \omega^*) = \epsilon(k, -\omega)$

$$\langle dE/dx \rangle = -\frac{2e^2}{\pi\beta^2} \int_0^{\infty} d\omega \int_{\omega/c\beta}^{\infty} dk \left[(\omega k) \left(\beta^2 - \frac{\omega^2}{k^2 c^2} \right) \text{Im} \left(\frac{1}{\epsilon\omega^2 - k^2 c^2} \right) + \frac{\omega}{kc^2} \text{Im} \left(\frac{1}{\epsilon} \right) \right]$$

The 1st term in the square bracket is from the vector potential (transverse) and vanishes at beta=0 while the 2nd term is from the scalar potential (longitudinal) and stays finite at beta=0. The energy loss is calculable when the complex dielectric constant is given. The formula suggests if the dielectric constant is real, there will be no energy loss.

The upper limit of the omega integral is of course finite in reality as constrained by kinematics:

$$\hbar\omega_{\max} = \frac{2m_e c^2 \beta^2 \gamma^2}{1 + 2\gamma (m_e/m) + (m_e/m)^2}$$

where m is the particle mass and m_e the electron mass.

Allison-Cobb (PAI) Model

All we need is the complex dielectric const.

$$\epsilon := \epsilon_1 + i\epsilon_2$$

Allison and Cobb relate its imaginary part to the photo-absorption cross section of the medium with

$$\epsilon_2(\omega) \simeq \frac{N}{Z} \left(\frac{c}{\omega} \right) \sigma_{\gamma}(\omega)$$

where N is the electron density of the medium and Z the atomic number of the molecule. They then get the real part of the dielectric constant with the Kramers-Kronig relation

$$\epsilon_1(\omega) - 1 = \frac{2}{\pi} \text{P} \int_0^{\infty} d\omega' \frac{\omega' \epsilon_2(\omega')}{\omega'^2 - \omega^2}$$

Indeed, we have

$$\begin{aligned} e^{ikx} &= e^{i(\text{Re } k + i \text{Im } k)x} \\ &= e^{i(\text{Re } k)x} e^{-(\text{Im } k)x} \\ &= e^{i(\text{Re } k)x} e^{-\frac{1}{2}(x/\lambda)} \end{aligned}$$

which together with

$$k = \sqrt{\epsilon} \omega / c$$

implies the attenuation length "lambda" to be given by

$$\begin{aligned} 1/\lambda \equiv 2 \text{Im } k &= 2(\omega/c) \text{Im } \sqrt{\epsilon} \\ &= 2(\omega/c) \text{Im} (\epsilon_1 + i\epsilon_2)^{1/2} \\ &\simeq (\omega/c) \epsilon_2 \end{aligned}$$

for a low density medium such as our TPC gas mixtures.

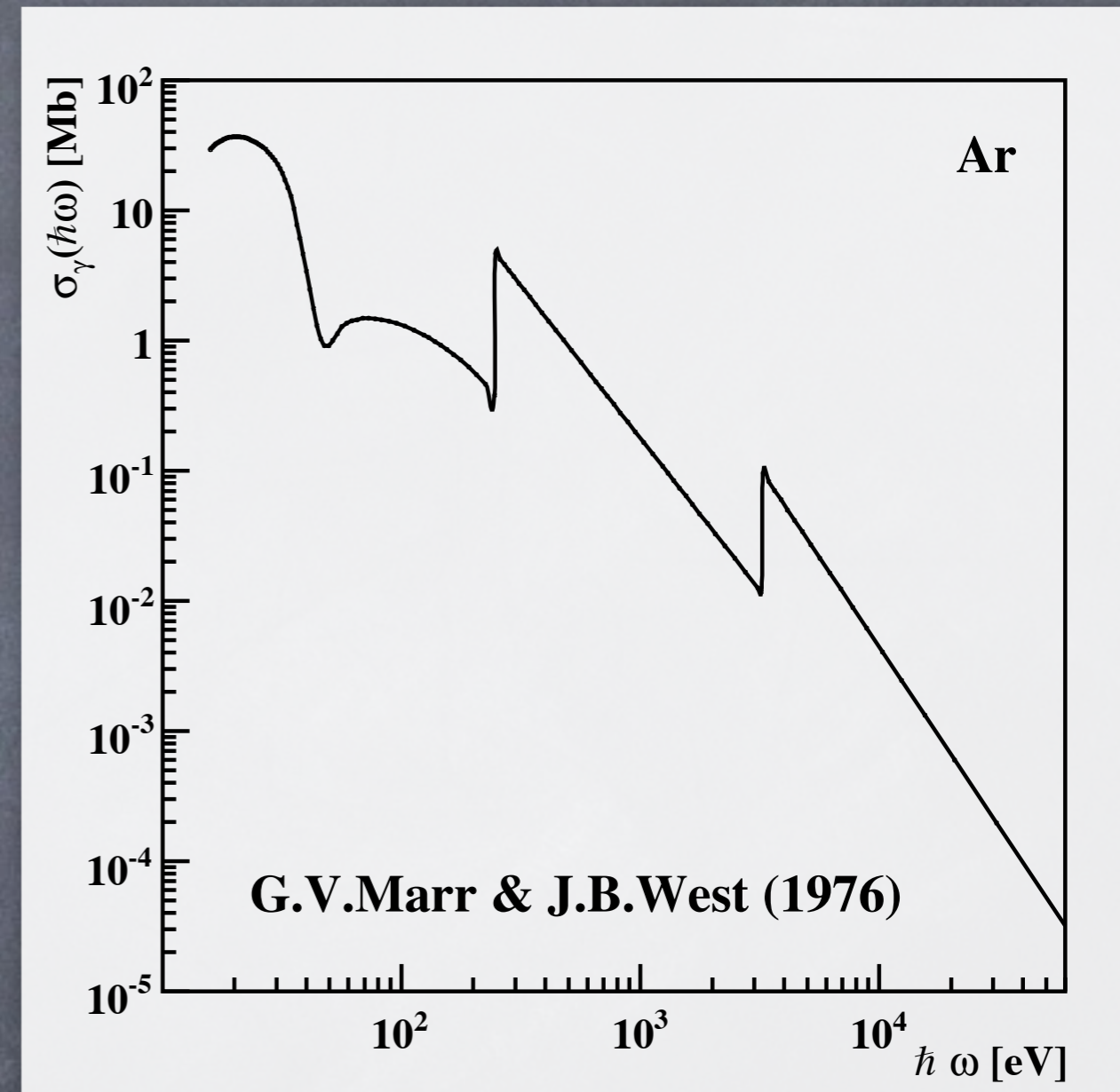
On the other hand, the attenuation length is related to the absorption cross section for photons:

$$\sigma_\gamma(\omega) = \frac{1}{(N/Z)\lambda}$$

leading us to

$$\epsilon_2(\omega) \simeq \frac{N}{Z} \left(\frac{c}{\omega} \right) \sigma_\gamma(\omega)$$

The photo-absorption cross section for Ar is shown below.

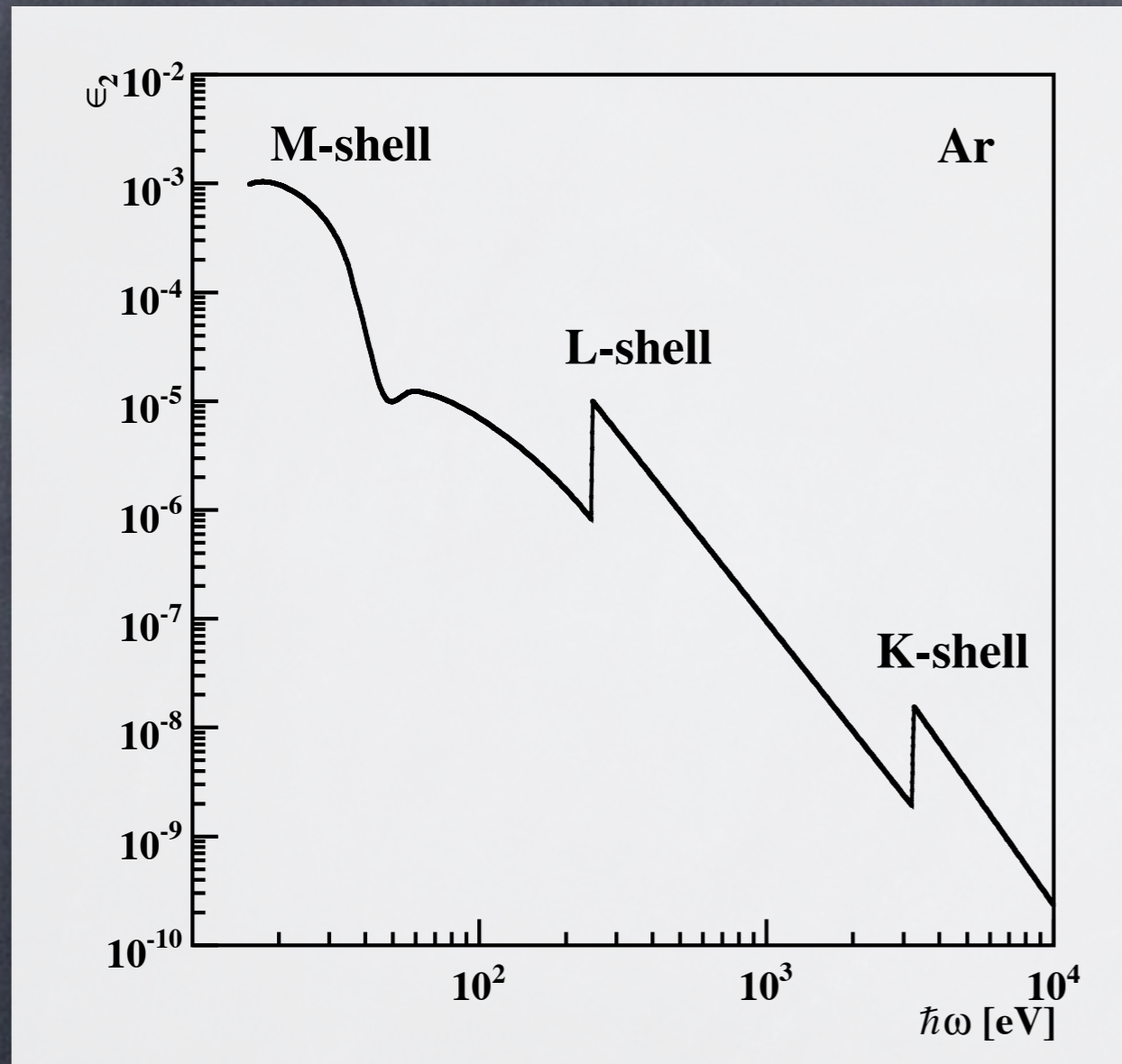


The cross section is roughly consistent with what you expect from the geometrical cross section of Ar:

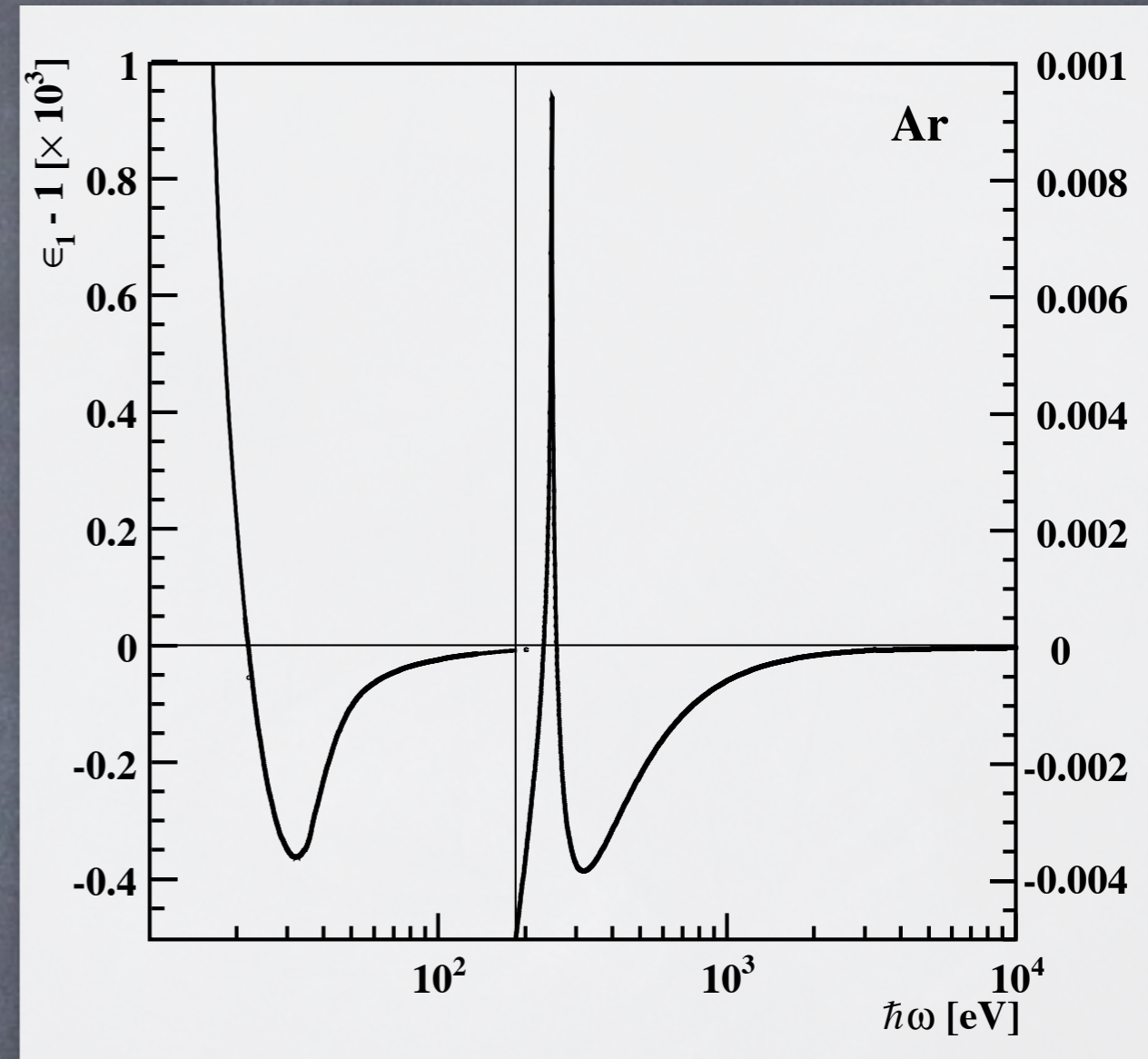
$$\pi(0.18 \text{ [nm]})^2 \times 8 \times \alpha_{\text{QED}} \simeq 58 \text{ [Mb]}$$

electrons in the outermost shell

The cross section can be translated into the imaginary part of the dielectric const. as shown in the next figure.



we obtain the real part as



where the region near the L-shell peak is zoomed up to show the resonance effect.

Using the Kramers-Kronig relation:

$$\epsilon_1(\omega) - 1 = \frac{2}{\pi} \text{P} \int_0^{\infty} d\omega' \frac{\omega' \epsilon_2(\omega')}{\omega'^2 - \omega^2}$$

These are, however, for real photons. The crucial step taken by Allison and Cobb was to extend this to virtual photons.

Kramers-Kronig Relation

Relation between Real and Imaginary Parts of Epsilon

Analyticity of Epsilon

The complex dielectric constant is analytic in the upper half omega plane as is seen from its definition

$$\epsilon(k, \omega) = 1 + \int_0^\infty d\tau \int_{|\xi| < c\beta\tau} d^3\xi G(|\xi|, \tau) e^{i(\mathbf{k}\cdot\xi - \omega\tau)}$$

It is real on the imaginary axis because of

$$\epsilon^*(k, \omega^*) = \epsilon(k, -\omega)$$

which is also easily derived from the above definition of the epsilon.

Recall also its asymptotic behavior

$$\epsilon(k, \omega) - 1 \simeq \frac{i\tilde{G}(0)}{\omega} - \frac{\tilde{G}'(0)}{\omega^2} + \dots = -\frac{\tilde{G}'(0)}{\omega^2} + \dots$$

with

$$\int_{|\xi| < c\beta\tau} d^3\xi G(|\xi|, \tau) e^{i\mathbf{k}\cdot\xi} \simeq \int_{|\xi| < c\beta\tau} d^3\xi G(|\xi|, \tau) = \tilde{G}(\tau)$$

The 1st term must vanish because of causality ($G=0$ for $\tau < 0$) and G 's continuity.

This shows that the integral of the epsilon over the upper semicircle vanishes. We can hence express the epsilon using Cauchy's integral:

$$\begin{aligned} \epsilon(\omega) - 1 &= \frac{1}{2\pi i} \int_{-\infty}^{+\infty} d\omega' \frac{\epsilon(\omega') - 1}{\omega' - \omega - i(+0)} \\ &= \frac{1}{2\pi i} \int_{-\infty}^{+\infty} d\omega' \left[\text{P} \frac{1}{\omega' - \omega} + i\pi \delta(\omega' - \omega) \right] (\epsilon(\omega') - 1) \\ &= \frac{1}{2\pi i} \text{P} \int_{-\infty}^{+\infty} d\omega' \frac{\epsilon(\omega') - 1}{\omega' - \omega} + \frac{1}{2} (\epsilon(\omega) - 1) \end{aligned}$$

Moving the last term of the R.H.S. to the L.H.S. we get

$$\epsilon(\omega) - 1 = \frac{1}{\pi i} \text{P} \int_{-\infty}^{+\infty} d\omega' \frac{\epsilon(\omega') - 1}{\omega' - \omega}$$

Taking the real parts of the both sides, dividing the integral path into -ve and +ve parts, and noting $\epsilon_2(-\omega) = -\epsilon_2(\omega)$ we have

$$\epsilon_1(\omega) - 1 = \frac{2}{\pi} \text{P} \int_0^\infty d\omega' \frac{\omega' \epsilon_2(\omega')}{\omega'^2 - \omega^2}$$

The Allison-Cobb Model

We have shown that the evaluation of the energy loss can be reduced to that of the imaginary part of the epsilon. As mentioned above, Allison and Cobb used the photo-absorption cross section to estimate the imaginary part. To show how, let us first introduce the general oscillator strength function "f" by

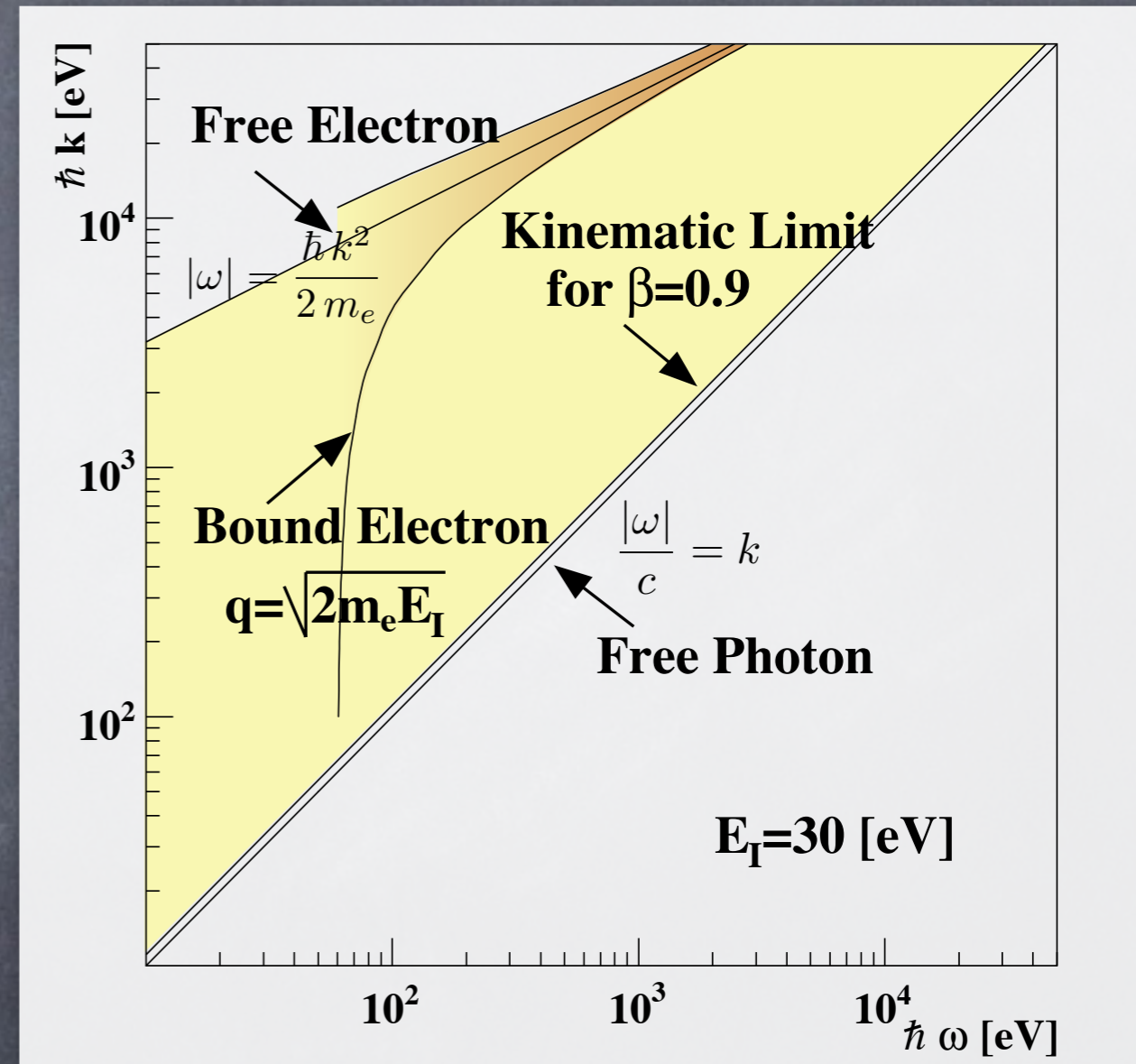
$$\epsilon_2(k, \omega) = \frac{2\pi^2 N e^2}{m_e \omega} f(k, \omega)$$

The general oscillator strength function is related to the dipole transition probability for absorption or emission of a photon. Since the epsilon_2 is an odd function of omega, the "f" is an even function of omega.

Since the imaginary part of the epsilon is related to the absorption cross section we can hence express the oscillator function in terms of the cross section

$$f(k, \omega) = \frac{m_e c}{2\pi^2 e^2 Z} \sigma_\gamma(|\omega|)$$

Strictly speaking, the formula is valid only for real photons. Allison and Cobb, however, assume that this holds approximately for even virtual photons, as long as they are below the free electron boundary.



The assumption implies that the "f" does not depend on "k" in the resonance region.

Allison and Cobb further assume that the contribution from the region above the free electron line can be approximated as a contribution entirely coming from this line. The assumption is equivalent to ignoring the momentum of bound electrons. This seems a rather crude approximation, but it works as they respect the Bethe sum rule:

$$\int_0^\infty f(k, \omega) d\omega = 1$$

and set

$$f(k, \omega) = \frac{m_e c}{2\pi^2 e^2 Z} \delta\left(|\omega| - \frac{\hbar k^2}{2m_e}\right) \int_0^{|\omega|} \sigma_\gamma(\omega') d\omega'$$

From classical point of view, the oscillator strength function counts the number of bound electrons in a molecule contributing to a particular oscillation mode with the frequency ω . The Bethe sum rule hence just dictates that the total number of bound electrons in the molecule is const.

Putting these together, we arrive at

$$\epsilon_2(k, \omega) = \frac{Nc}{\omega Z} \left[\sigma_\gamma(|\omega|) \theta\left(|\omega| - \frac{\hbar k^2}{2m_e}\right) + \int_0^{|\omega|} \sigma_\gamma(\omega') d\omega' \delta\left(|\omega| - \frac{\hbar k^2}{2m_e}\right) \right]$$

Now all we need to do is to put this into the dE/dx formula

$$\langle dE/dx \rangle = -\frac{2e^2}{\pi\beta^2} \int_0^\infty d\omega \int_{\omega/c\beta}^\infty dk \left[(\omega k) \left(\beta^2 - \frac{\omega^2}{k^2 c^2} \right) \text{Im} \left(\frac{1}{\epsilon\omega^2 - k^2 c^2} \right) + \frac{\omega}{k c^2} \text{Im} \left(\frac{1}{\epsilon} \right) \right]$$

and carry out integrations. Since the 1st term in the square bracket is dominated by the resonance region due to the pole of the propagator, we can set

$$\epsilon_2(k, \omega) \approx \frac{Nc}{\omega Z} \sigma_\gamma(|\omega|)$$

Since there is no k -dependence here, the k -integral is now straightforward. As for the 2nd term in the square bracket, since it is dominated by the nearly free electron region, and since we are dealing with a low density material ($|\epsilon| \simeq 1$), we can set

$$\text{Im} \left(\frac{1}{\epsilon} \right) = -\frac{\epsilon_2}{|\epsilon|} \simeq -\epsilon_2(k, \omega)$$

The Allison-Cobb Formula

With these approximations, we can carry out the integrations in an elementary way and obtain

$$\langle dE/dx \rangle = \frac{e^2}{\pi\beta^2 c^2} \int_0^\infty d\omega \left[\frac{Nc}{Z} \sigma_\gamma(\omega) \ln \left[(1 - \epsilon_1\beta^2)^2 + (\epsilon_2\beta^2)^2 \right]^{-\frac{1}{2}} \right. \\ \left. + \omega \left(\beta^2 - \frac{\epsilon_1}{|\epsilon|^2} \right) \text{atan} \left(\frac{\epsilon_2\beta^2}{1 - \epsilon_1\beta^2} \right) \right. \\ \left. + \frac{Nc}{Z} \sigma_\gamma(\omega) \ln \left(\frac{2m_e\beta^2 c^2}{\hbar\omega} \right) \right. \\ \left. + \frac{Nc}{\omega} \int_0^\omega \frac{\sigma_\gamma(\omega')}{Z} d\omega' \right]$$

with

$$\epsilon_2(\omega) = \frac{Nc}{\omega Z} \sigma_\gamma(|\omega|)$$

and the Kramers-Kronig relation

$$\epsilon_1(\omega) - 1 = \frac{2}{\pi} \text{P} \int_0^\infty d\omega' \frac{\omega' \epsilon_2(\omega')}{\omega'^2 - \omega^2}$$

The Differential Cross Section

We can reinterpret the average energy loss formula as from discrete collisions of the particle with a bound electron exchanging a virtual photon with an energy $\hbar\omega$.

Denoting the differential cross section for the particle hitting the bound electron with the virtual photon by $d\sigma$, we can write

$$\left\langle \frac{dE}{dx} \right\rangle = \int_0^\infty N(\hbar\omega) \frac{d\sigma}{d(\hbar\omega)} d(\hbar\omega)$$

Since there is no fear for confusion, we put

$$E = \hbar\omega$$

and compare this with the Allison-Cobb formula. We then obtain

$$\frac{d\sigma}{dE} = \frac{\alpha}{\pi\beta^2} \left[\frac{\sigma_\gamma(E)}{E Z} \ln \left[(1 - \epsilon_1\beta^2)^2 + (\epsilon_2\beta^2)^2 \right]^{-\frac{1}{2}} \right. \\ \left. + \frac{1}{Nc\hbar} \left(\beta^2 - \frac{\epsilon_1}{|\epsilon|^2} \right) \text{atan} \left(\frac{\epsilon_2\beta^2}{1 - \epsilon_1\beta^2} \right) \right. \\ \left. + \frac{\sigma_\gamma(E)}{E Z} \ln \left(\frac{2m_e\beta^2 c^2}{E} \right) \right. \\ \left. + \frac{1}{E^2} \int_0^E \frac{\sigma_\gamma(E')}{Z} dE' \right]$$

The 1st and 2nd lines on the R.H.S. are from the vector potential (transverse photons) and the 3rd and 4th lines from the scalar potential (longitudinal photons).

The Beta Dependence

The transverse cross section vanishes in the beta→0 limit, while the longitudinal cross section behaves as 1/beta².

On the other hand, in the beta→1 limit, the longitudinal cross section becomes const.

The 2nd term becomes important in this limit and is related to the emissions of Cherenkov photons. As a matter of fact, recalling that and $\epsilon_2 \ll 1$ $|\epsilon_1 - 1| \ll 1$ for a low density medium, we notice that below and above $\beta = 1/\sqrt{\epsilon_1}$

$$\text{atan} \left(\frac{\epsilon_2 \beta^2}{1 - \epsilon_1 \beta^2} \right) \simeq 0 \rightarrow \pi$$

Above, the 2nd term becomes

$$N \frac{d\sigma_C}{d\omega} \simeq \frac{\alpha}{c} \left(1 - \frac{1}{\epsilon_1(\omega) \beta^2} \right)$$

which is none other than the well known frequency distribution of the Cherenkov radiation.

The rest of the cross section can be put together and cast into the form

$$\begin{aligned} \frac{d\sigma_{NC}}{dE} &= \frac{\alpha}{\pi\beta^2} \left[\frac{\sigma_\gamma(E)}{E Z} \ln \frac{\beta^2}{\left[(1 - \epsilon_1 \beta^2)^2 + (\epsilon_2 \beta^2)^2 \right]^{\frac{1}{2}}} \right. \\ &\quad \left. + \frac{\sigma_\gamma(E)}{E Z} \ln \left(\frac{2m_e c^2}{E} \right) + \frac{1}{E^2} \int_0^E \frac{\sigma_\gamma(E')}{Z} dE' \right] \\ &= \frac{a}{\beta^2} \left[\ln \frac{\beta^2}{\left[(1 - \epsilon_1 \beta^2)^2 + (\epsilon_2 \beta^2)^2 \right]^{\frac{1}{2}}} + b \right] \\ &= a \frac{1 + (\beta\gamma)^2}{(\beta\gamma)^2} \left[\ln \frac{(\beta\gamma)^2}{\left[(1 + (1 - \epsilon_1)(\beta\gamma)^2)^2 + (\epsilon_2(\beta\gamma)^2)^2 \right]^{\frac{1}{2}}} + b \right] \end{aligned}$$

The cross section hence behaves as

$$\frac{d\sigma_{NC}}{dE} \simeq a \frac{1 + (\beta\gamma)^2}{(\beta\gamma)^2} [\ln(\beta\gamma)^2 + b]$$

where $|\epsilon_1 - 1| (\beta\gamma)^2 \ll 1$ and $\epsilon_2 (\beta\gamma)^2 \ll 1$. The conditions hold over a rather wide range for a low density medium with $|\epsilon_1 - 1| \ll 1$.

In the relativistic region where

$$1 \ll (\beta\gamma)^2 \ll 1/|\epsilon - 1|$$

the X-section thus shows **the relativistic rise**

$$\frac{d\sigma_{NC}}{dE} \simeq 2a \ln(\gamma) + ab$$

The relativistic rise comes from the fact that in the $\beta \rightarrow 1$ limit the virtual photon gets closer to the real photon pole of the propagator and hence acquires a longer range, resulting in a larger cross section. This rise, however, saturates where

$$(\beta\gamma)^2 \gg 1/|\epsilon - 1|$$

and reaches an asymptotic value

$$\frac{d\sigma_{NC}}{dE} \simeq a \ln |\epsilon - 1|^{-1} + ab$$

The saturation due to a finite density of the medium is called **the density effect**.

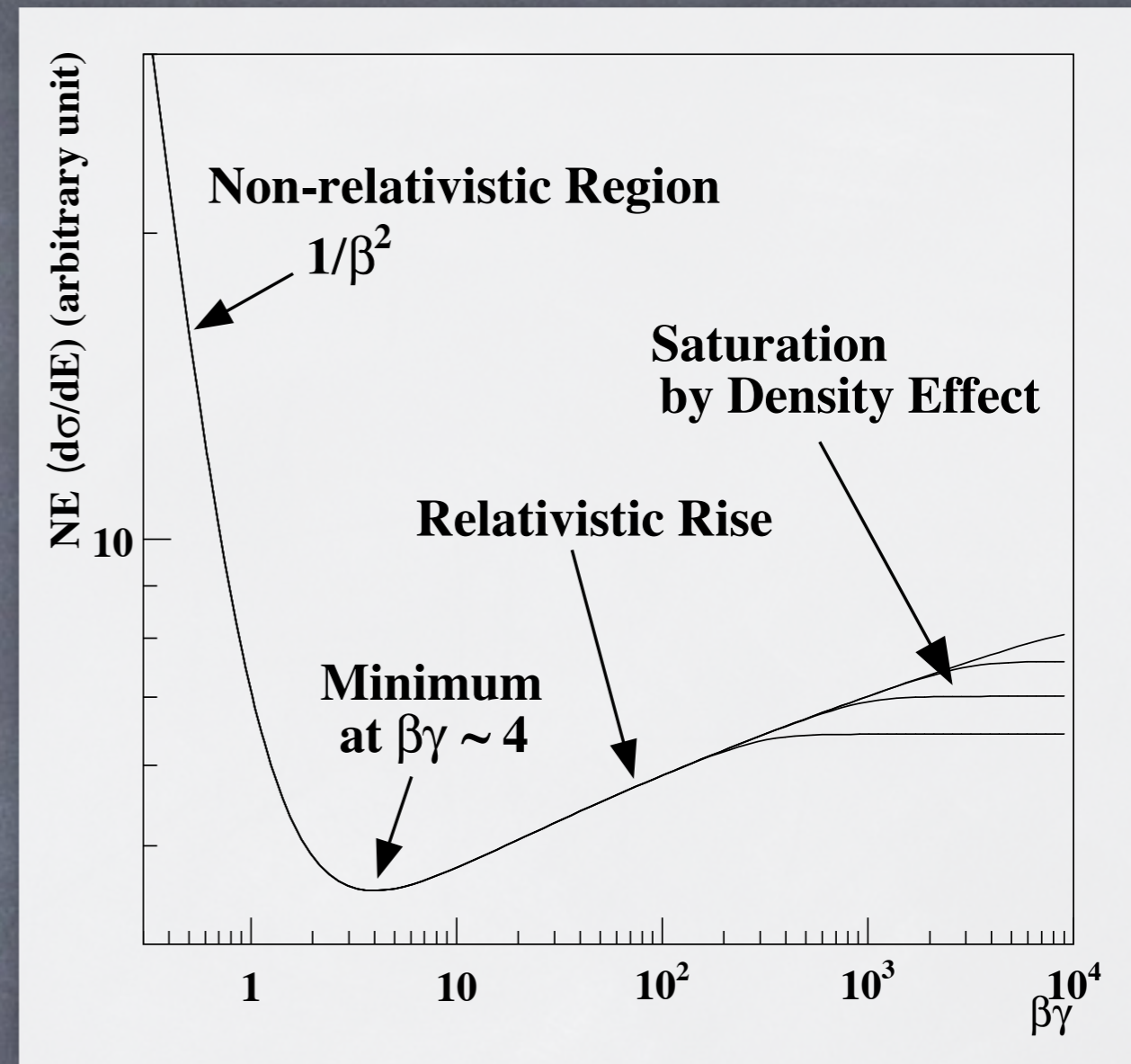
The saturation sets in when

$$2 \ln \gamma \simeq \ln |\epsilon - 1|^{-1}$$

or when

$$\gamma \simeq \gamma^* := \frac{1}{\sqrt{|1 - \epsilon|}}$$

It is worth remembering that the minimum occurs at around $\beta\gamma \sim 4$ with almost no dependence on the medium.



It should also be noted that the saturation depends on the photon energy. In the free electron region (high omega limit), we have

$$\epsilon = 1 - \frac{4\pi N e^2}{m_e \omega^2} := 1 - \frac{\omega_p^2}{\omega^2} < 1$$

where the plasma frequency is given by

$$\omega_p^2 := 4\pi N e^2 / m_e$$

In this high frequency or high E region, the gamma* is given by

$$\gamma^* \simeq \frac{\omega}{\omega_p} = \left(\frac{m_e}{4\pi N e^2} \right)^{1/2} \frac{E}{\hbar}$$

The higher the energy, the larger the gamma at which the saturation sets in.

The Energy Transfer / Collision

For a low E, the resonance region dominates and hence the 1st and the 3rd terms of

$$\begin{aligned} \frac{d\sigma}{dE} = \frac{\alpha}{\pi\beta^2} & \left[\frac{\sigma_\gamma(E)}{E Z} \ln \left[(1 - \epsilon_1\beta^2)^2 + (\epsilon_2\beta^2)^2 \right]^{-\frac{1}{2}} \right. \\ & + \frac{1}{Nc\hbar} \left(\beta^2 - \frac{\epsilon_1}{|\epsilon|^2} \right) \text{atan} \left(\frac{\epsilon_2\beta^2}{1 - \epsilon_1\beta^2} \right) \\ & + \frac{\sigma_\gamma(E)}{E Z} \ln \left(\frac{2m_e\beta^2 c^2}{E} \right) \\ & \left. + \frac{1}{E^2} \int_0^E \frac{\sigma_\gamma(E')}{Z} dE' \right] \end{aligned}$$

give a major contribution. The E spectrum hence reflects the resonance structures of the photo-absorption cross section.

At high E values, only a quasi-free electron region will be kinematically allowed, and hence the 4th term determines the trend.

$$\frac{d\sigma}{dE} \rightarrow \frac{\alpha}{\pi\beta^2} \frac{1}{E^2} \int_0^E \frac{\sigma_\gamma(E')}{Z} dE'$$

Recalling the relation between the cross section and the oscillator strength and the Bethe sum rule, we have

$$\frac{d\sigma}{dE} \rightarrow \frac{2\pi e^4}{m_e c^2} \frac{1}{\beta^2 E^2} = \frac{e^2}{c^2 \beta^2} \frac{\omega_p^2}{2 N E^2}$$

This is the Rutherford scattering formula. The formula indicates that the delta-ray production has a long tail characterized by $1/E^2$ behavior.

There is of course a kinematical limit to set the maximum energy transfer, but this limit is practically never reached since such energetic collisions create delta electrons which will make separate tracks.

The Bethe-Bloch Formula

Relation between Allison-Cobb and Bethe-Bloch

The Decomposition to T/L Parts

The dE/dx formula can be separated into the transverse and the longitudinal parts

$$\left\langle \frac{dE}{dx} \right\rangle = \left\langle \frac{dE}{dx} \right\rangle_T + \left\langle \frac{dE}{dx} \right\rangle_L$$

Let us now examine them separately.

The Transverse Part

The transverse part is given by

$$\left\langle \frac{dE}{dx} \right\rangle_T = \frac{e^2}{(2\pi) c^2 \beta^2 i} \int_{-\infty}^{+\infty} d\omega \omega \int_{(\omega/c\beta)^2}^{\infty} dk^2 \left(\frac{\beta^2 k^2 c^2 - \omega^2}{k^2 c^2 - \epsilon(\omega) \omega^2} \right) \frac{1}{k^2}$$

Replacing the complex dielectric constant by the Allison-Cobb model led us to the Allison Cobb formula. This time we will try to carry out the integrations directly. We assume that the epsilon does not depend on k following Allison and Cobb. The k -integral is then straightforward:

$$\left\langle \frac{dE}{dx} \right\rangle_T = \frac{e^2}{(2\pi) c^2 \beta^2 i} \int_{-\infty}^{+\infty} d\omega \omega \left(\beta^2 - \frac{1}{\epsilon(\omega)} \right) \ln \left(\frac{1}{1 - \beta^2 \epsilon(\omega)} \right)$$

To proceed further, we will make full use of the analyticity of the epsilon in the upper half omega plane. We will try to move the integration path to the upper semicircle, since the epsilon reaches its asymptotic form there:

$$\epsilon(\omega) \rightarrow 1 - \frac{\omega_p^2}{\omega^2}$$

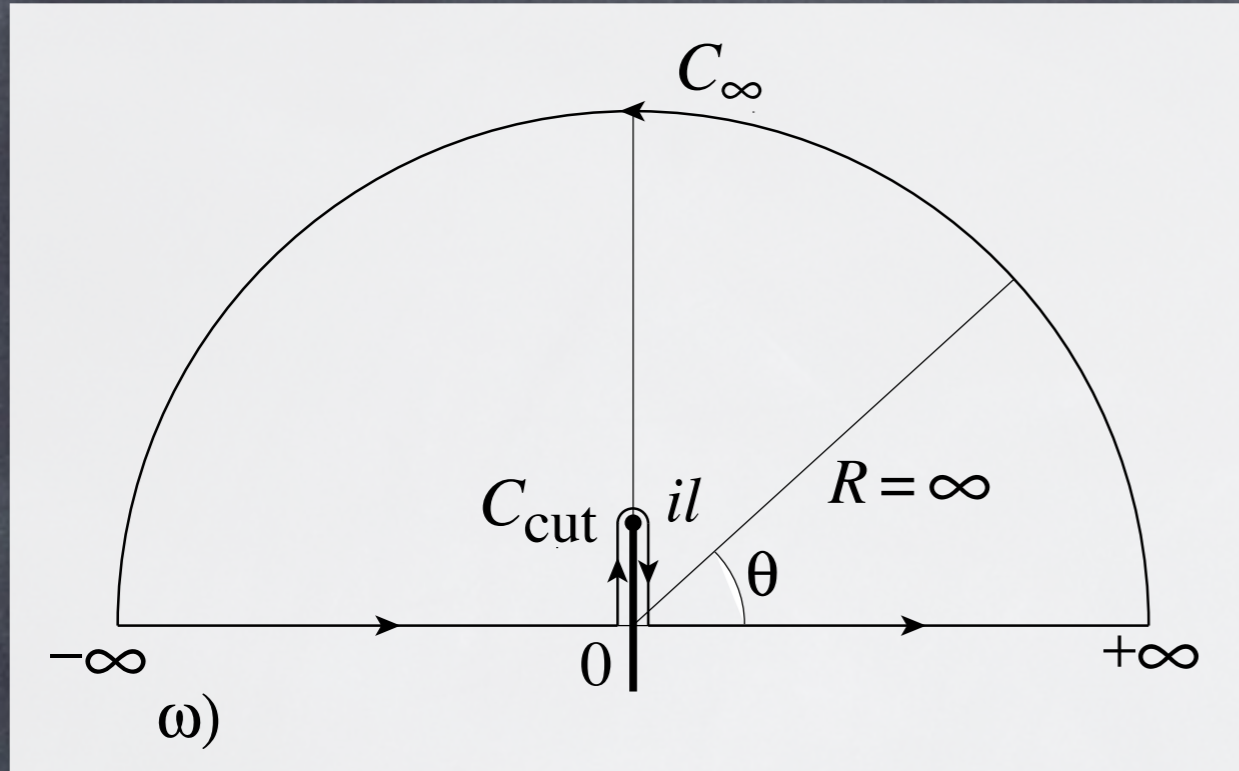
and hence we can carry out the integration. There is, however, a cut on the imaginary axis if

$$1 - \beta^2 \epsilon(0) < 0$$

In this case, the discontinuity across this cut contributes to the integration along the real axis, too. We thus split the integral as

$$\left\langle \frac{dE}{dx} \right\rangle_T = \left\langle \frac{dE}{dx} \right\rangle_{-C_\infty} - \left\langle \frac{dE}{dx} \right\rangle_{C_{\text{cut}}}$$

where we defined the integration paths as in the following figure:



The upper semicircle gives

$$\begin{aligned} \left\langle \frac{dE}{dx} \right\rangle_{-C_\infty} &= \frac{e^2}{(2\pi) c^2 \beta^2 i} \int_{-C_\infty} d\omega \omega \left(\beta^2 - \frac{1}{\epsilon(\omega)} \right) \ln \left(\frac{1}{1 - \beta^2 \epsilon(\omega)} \right) \\ &= \frac{e^2}{(2\pi) c^2 \beta^2 i} \int_{-C_\infty} d\omega \omega \left(\beta^2 - \frac{1}{1 - \omega_p^2/\omega^2} \right) \ln \left(\frac{1}{1 - \beta^2 (1 - \omega_p^2/\omega^2)} \right) \\ &= \frac{e^2}{2 c^2 \beta^2} \omega_p^2 \left[\ln \left(\frac{1}{1 - \beta^2} \right) - \beta^2 \right] \end{aligned}$$

In the low density limit, since there exists no cut, this gives the total transverse contribution, which is entirely specified by the plasma frequency of the medium.

For a high beta value, the cut shows up and we have

$$\begin{aligned} \left\langle \frac{dE}{dx} \right\rangle_{C_{\text{cut}}} &= \frac{e^2}{(2\pi) c^2 \beta^2 i} \int_{C_{\text{cut}}} d\omega \omega \left(\beta^2 - \frac{1}{\epsilon(\omega)} \right) \ln \left(\frac{1}{1 - \beta^2 \epsilon(\omega)} \right) \\ &= -\frac{e^2}{(2\pi) c^2 \beta^2 i} \int_0^l d\zeta \zeta \left(\beta^2 - \frac{1}{\epsilon(i\zeta)} \right) \left[\ln \left(\frac{1}{1 - \beta^2 \epsilon(-\delta + i\zeta)} \right) - \ln \left(\frac{1}{1 - \beta^2 \epsilon(+\delta + i\zeta)} \right) \right] \end{aligned}$$

and hence

$$\left\langle \frac{dE}{dx} \right\rangle_{C_{\text{cut}}} = \frac{e^2}{c^2 \beta^2} \int_0^l d\zeta \zeta \left(\beta^2 - \frac{1}{\epsilon(i\zeta)} \right)$$

This represents the density effect. Putting these together, we arrive at

$$\left\langle \frac{dE}{dx} \right\rangle_T = \frac{e^2}{c^2 \beta^2} \left\{ \frac{1}{2} \omega_p^2 \left[\ln \left(\frac{1}{1 - \beta^2} \right) - \beta^2 \right] - \int_0^l d\zeta \zeta \left(\beta^2 - \frac{1}{\epsilon(i\zeta)} \right) \right\}$$

The formula corresponds to the 1st and the 2nd terms of the Allison-Cobb formula.

The Longitudinal Part

The longitudinal part is given by

$$\left\langle \frac{dE}{dx} \right\rangle_L = \frac{e^2}{(2\pi) c^2 \beta^2 i} \int_{-\infty}^{+\infty} d\omega \omega \int_{(\omega/c\beta)^2}^{\infty} dk^2 \left(-\frac{1}{k^2 \epsilon(\omega)} \right)$$

Slightly going off the Allison-Cobb model we assume that epsilon is k-independent.

We carry out the k-integration to get

$$\begin{aligned} \left\langle \frac{dE}{dx} \right\rangle_L &= \frac{e^2}{(2\pi) c^2 \beta^2 i} \int_{-\infty}^{+\infty} \left(-\frac{\omega d\omega}{\epsilon(\omega)} \right) \int_{(\omega/c\beta)^2}^{\infty} \frac{dk^2}{k^2} \\ &= \frac{e^2}{\pi c^2 \beta^2} \text{Im} \int_0^{+\infty} \left(-\frac{\omega d\omega}{\epsilon(\omega)} \right) \ln \left(\frac{k_{\max}^2 c^2 \beta^2}{\omega^2} \right) \end{aligned}$$

We recall here that epsilon becomes real in the omega->0 limit. This means that for the epsilon to acquire an imaginary part, there must be photon absorption that in turn requires some finite amount of energy to excite the lowest level. There must hence be a lower limit to the omega range of the integration as well as to the k-integration range.

Noting that

$$-\text{Im} \int_0^{\infty} \frac{\omega d\omega}{\epsilon(\omega)} = \frac{1}{2} \int_{-\infty}^{+\infty} \frac{i \omega d\omega}{\epsilon(\omega)} = \frac{1}{2} \int_{-c\infty}^{\infty} \frac{i \omega d\omega}{1 - \omega_p^2/\omega^2} = \frac{\pi}{2} \omega_p^2$$

we introduce such a limit on the k-integral with a frequency $\bar{\omega}$ defined by

$$\text{Im} \int_0^{+\infty} \left(-\frac{\omega d\omega}{\epsilon(\omega)} \right) \ln(\hbar\omega) \equiv \frac{\pi}{2} \omega_p^2 \ln I \equiv \frac{\pi}{2} \omega_p^2 \ln(\hbar\bar{\omega})$$

where "I" is the effective binding energy.

Recalling the kinematic relation

$$\hbar\omega_{\max} = \frac{2m_e c^2 \beta^2 \gamma^2}{1 + 2\gamma (m_e/m) + (m_e/m)^2}$$

we have

$$(\hbar k_{\max})^2 \simeq 2m_e \hbar\omega_{\max} = 2m_e T_{\max}$$

With these, we arrive at

$$\left\langle \frac{dE}{dx} \right\rangle_L = \frac{e^2}{c^2 \beta^2} \frac{1}{2} \omega_p^2 \ln \left(\frac{2m_e c^2 \beta^2 T_{\max}}{I^2} \right)$$

that corresponds to the 3rd and 4th terms (longitudinal part) of the Allison-Cobb formula.

The Bethe-Bloch Formula

Putting the T and L parts together, we get

$$\begin{aligned} \left\langle \frac{dE}{dx} \right\rangle &= \frac{e^2}{c^2 \beta^2} \left\{ \frac{1}{2} \omega_p^2 \left[\ln \left(\frac{2m_e c^2 \beta^2 T_{\max}}{I^2} \right) + \ln \left(\frac{1}{1 - \beta^2} \right) - \beta^2 \right] \right. \\ &\quad \left. - \int_0^l d\zeta \zeta \left(\beta^2 - \frac{1}{\epsilon(i\zeta)} \right) \right\} \end{aligned}$$

with

$$\omega_p^2 := 4\pi N e^2 / m_e$$

and

$$T_{\max} = \hbar\omega_{\max} \simeq 2m_e c^2 \beta^2 \gamma^2$$

The dE/dx Fluctuation

Energy loss per a finite sample thickness

The General Formula

Let x be a finite sample thickness and Δ be the corresponding energy loss.

What we need is a probability distribution function: $F(x, \Delta)$. The distribution must satisfy the following equation

$$F(x + \delta x, \Delta) = F(x, \Delta) \left[1 - \int_0^\infty N \left(\delta x \frac{d\sigma(E)}{dE} \right) dE \right] + \int_0^\infty F(x, \Delta - E) N \left(\delta x \frac{d\sigma(E)}{dE} \right) dE$$

where the 1st term on the R.H.S. is the probability of losing Δ in the first x and then nothing happening in the next δx , while the 2nd term on the R.H.S. gives the sum of the probabilities of losing $\Delta - E$ in the first x and E in the subsequent δx .

This leads us to the following equation

$$\frac{\partial F(x, \Delta)}{\partial x} = \int_0^\infty N \left(\frac{d\sigma(E)}{dE} \right) [F(x, \Delta - E) - F(x, \Delta)] dE$$

By making Laplace transform

$$\bar{F}(x, s) = \int_0^\infty d\Delta F(x, \Delta) e^{-s\Delta}$$

$$F(x, \Delta) = \frac{1}{2\pi i} \int_{-i\infty+\sigma}^{+i\infty+\sigma} ds \bar{F}(x, s) e^{s\Delta}$$

we obtain

$$\frac{\partial \bar{F}(x, s)}{\partial x} = -\bar{F}(x, s) \int_0^\infty dE N \left(\frac{d\sigma(E)}{dE} \right) (1 - e^{-sE})$$

with the boundary condition

$$\bar{F}(0, s) = 1$$

corresponding to its original form:

$$F(0, \Delta) = \delta(\Delta)$$

The equation is readily solved to yield

$$\bar{F}(x, s) = \exp \left[-x \int_0^\infty dE N \left(\frac{d\sigma(E)}{dE} \right) (1 - e^{-sE}) \right]$$

By inverse Laplace transformation, we get

$$F(x, \Delta) = \frac{1}{2\pi i} \int_{-i\infty+\sigma}^{+i\infty+\sigma} ds \exp [s \Delta - x \int_0^\infty dE N \left(\frac{d\sigma(E)}{dE} \right) (1 - e^{-sE})]$$

This is a general solution. In principle we can numerically calculate the probability distribution once a concrete expression is given for the differential X-section (e.g. the Allison-Cobb). Landau analytically did the integral with the Rutherford scattering cross section.

Landau Distribution

Let E_0 be a characteristic energy (of the order of average binding energy) of atoms in the medium and E_{\max} be the maximum energy transfer from the particle to an electron in the medium. Landau assumed that the integral in the exponent comes only from the region

$$1/E_{\max} \ll s \ll 1/E_0$$

We will discuss physical meanings of this assumption later. The assumption ensures that we can always choose E_1 in such a way that

$$E_0 \ll E_1 \ll 1/s$$

Then we can separate the integral into two parts $(0, E_1)$ and (E_1, ∞) , and in the first we can make approximation

$$1 - e^{sE} \simeq -sE$$

to obtain

$$\int_0^\infty \left(\frac{d\sigma(E)}{dE} \right) (1 - e^{-sE}) dE = s \int_0^{E_1} dE \left(\frac{d\sigma(E)}{dE} \right) E + \int_{E_1}^\infty dE \left(\frac{d\sigma(E)}{dE} \right) (1 - e^{-sE})$$

Recalling the Rutherford formula

$$\frac{d\sigma}{dE} = \frac{2\pi e^4}{m_e c^2 \beta^2} \frac{1}{E^2}$$

we obtain for the 1st term

$$\int_0^{E_1} dE \left(\frac{d\sigma(E)}{dE} \right) E = \frac{2\pi e^4}{m_e c^2 \beta^2} \ln \left(\frac{E_1}{E'} \right)$$

where we choose the lower limit of the integral so as to reproduce the Bethe-Bloch

$$\ln E' = \ln \frac{I^2}{2m_e c^2 \beta^2 \gamma^2} + \beta^2$$

In this way, we can take the bound electron effects approximately.

On the other hand, the 2nd term can be partially integrated to give

$$\begin{aligned} \int_{E_1}^{\infty} dE \frac{1 - e^{-sE}}{E^2} &= \frac{1}{E_1} (1 - e^{-sE_1}) + s \int_{E_1}^{\infty} dE \frac{e^{-sE}}{E} \\ &\simeq s \left(1 + \int_{E_1}^{\infty} dE \frac{e^{-sE}}{E} \right) \end{aligned}$$

Again using $sE_1 \ll 1$, we have

$$\begin{aligned} \int_{E_1}^{\infty} dE \frac{e^{-sE}}{E} &= \int_{sE_1}^{\infty} dz \frac{e^{-z}}{z} \\ &= \int_{sE_1}^1 \frac{dz}{z} + \int_{sE_1}^1 dz \frac{e^{-z} - 1}{z} + \int_1^{\infty} dz \frac{e^{-z}}{z} \\ &\simeq \int_{sE_1}^1 \frac{dz}{z} + \int_0^1 dz \frac{e^{-z} - 1}{z} + \int_1^{\infty} dz \frac{e^{-z}}{z} \\ &= \int_{sE_1}^1 \frac{dz}{z} - \gamma_E \end{aligned}$$

where the Euler constant is

$$\gamma_E \simeq 0.577$$

The 2nd term now becomes

$$\int_{E_1}^{\infty} dE \frac{1 - e^{-sE}}{E^2} = s (1 - \gamma_E - \ln sE_1)$$

Putting the 1st and 2nd terms together, we arrive at

$$x N \int_0^{\infty} dE \left(\frac{d\sigma}{dE} \right) (1 - e^{-sE}) = \xi s (1 - \gamma_E - \ln sE')$$

with

$$\xi := x \frac{2\pi N e^4}{m_e c^2 \beta^2}$$

Introducing a dimensionless scaling variable

$$\eta(\xi, \Delta) := \frac{\Delta - \xi \left(\ln \frac{\xi}{E'} + 1 - \gamma_E \right)}{\xi}$$

we finally arrive at

$$F(x, \Delta) = \frac{1}{\xi} \frac{1}{2\pi i} \int_{-i\infty+\sigma}^{+i\infty+\sigma} du e^{u \ln u + \eta u} =: \frac{1}{\xi} \phi(\eta)$$

The universal function $\phi(\eta)$ attains its maximum of about 0.18 at

$$\eta = \eta_{\text{MPV}} \simeq -0.05$$

It has a FWHM of about 4, suggesting that ξ sets the scale of energy loss.

Region of Applicability

Let us now examine the approximation we made to derive the Landau distribution and clarify the region of applicability.

Inspection of

$$\phi(\eta) := \frac{1}{2\pi i} \int_{-i\infty+\sigma}^{+i\infty+\sigma} du e^{u \ln u + \eta u}$$

tells us that the major contribution comes from the region where $\ln u \sim 0$ or $u \sim 1$. The assumption for the important "s" region

$$1/E_{\max} \ll s \ll 1/E_0$$

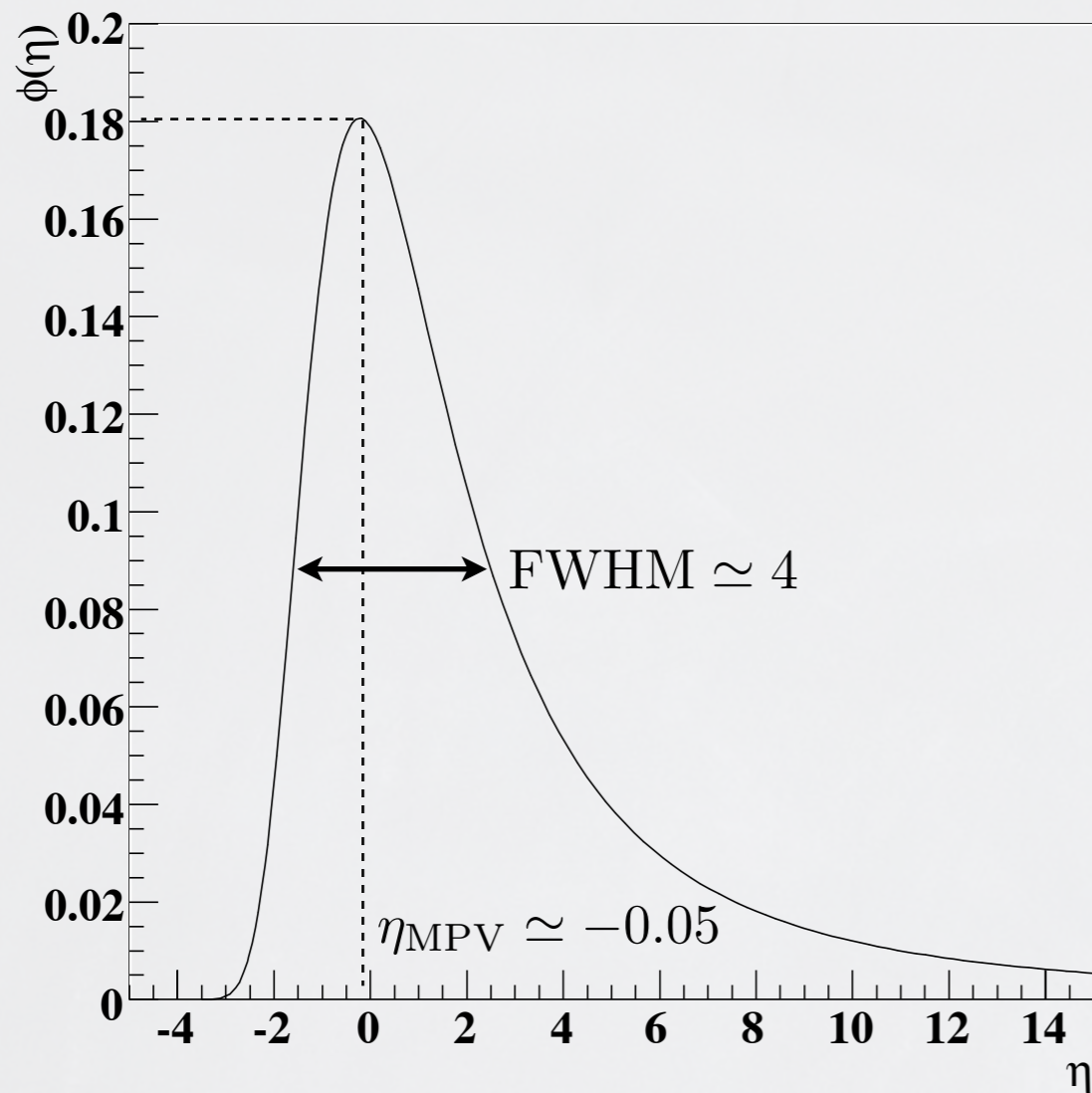
can hence be translated to

$$sE_0 = \frac{u}{\xi} E_0 \sim \frac{E_0}{\xi} \ll 1 \quad \text{and} \quad sE_{\max} = \frac{u}{\xi} E_{\max} \sim \frac{E_{\max}}{\xi} \gg 1$$

or equivalently

$$E_0 \ll \xi := x \frac{2\pi N e^4}{m_e c^2 \beta^2} \ll E_{\max} \simeq 2m_e c^2 \beta^2 \gamma^2$$

It says that the medium must be thick enough for "xi" to be much larger than the binding energy scale, while it must be thin enough to be much less than the maximum energy transfer per collision.



The Most Probable Value (MPV) position is

$$\begin{aligned} \Delta = \Delta_{\text{MPV}} &:= \xi \left(\ln \frac{\xi}{E'} + 1 - \gamma_E + \eta_{\text{MPV}} \right) \\ &= \left(\frac{2\pi N e^4}{m_e c^2 \beta^2} x \right) \left[\ln \left(\frac{4\pi N e^4 \gamma^2 x}{I^2} \right) - \beta^2 + 1 - \gamma_E + \eta_{\text{MPV}} \right] \end{aligned}$$

which shows roughly the same beta dependence as the Bethe-Bloch formula.

Comparison with Data

Allison-Cobb (1980)

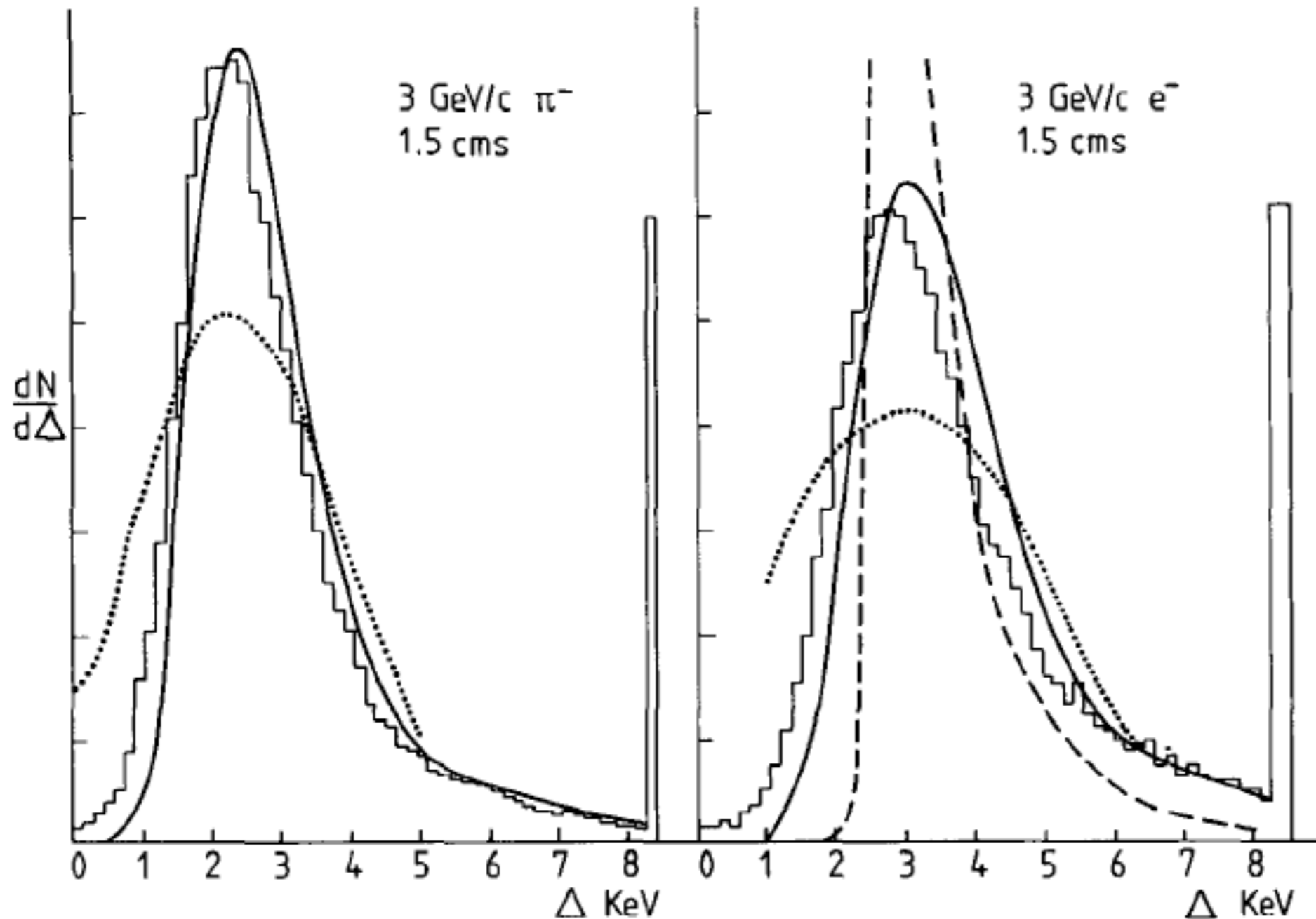


Figure 9 Experimental energy-loss distributions of Harris et al (1973) for π and e at 3 GeV/c in 1.5 cm of argon/7% CH₄ at normal density. The dashed and dotted curves are calculations using the model of Landau (1944) with corrections of Maccabee & Papworth (1969) and Blunck & Leisegang (1950) respectively. The solid curves are the predictions of the PAI model.

The energy loss

$$\Delta = n_I W$$

ionization
electrons

Average energy
for creation of 1
electron

Some numbers to
remember

$$W_{\text{Ar}} = 26 \text{ [eV]}$$

$$n_I(1 \text{ [cm] Ar}) \simeq 100$$

$$\frac{\# \text{ primary clusters}}{1 \text{ [cm] of Ar}} \simeq 30$$

Cluster Size Distribution

The number of electrons per cluster

Charge Size

Depending on the number of electrons made by 2ndary ionizations, each primary cluster has different number of electrons in it. Its distribution function is not easy to calculate from the 1st principle, since the number of electrons per cluster is typically a few and hence its statistical treatment as with the number of ionization electrons per a finite sampling thickness is inadequate.

What we actually measure with a TPC is usually the charge collected on a pad with a finite size. Individual primary clusters seem not to be our concern. This is, however, certainly wrong for pixel readout. Even for conventional pad readout, the cluster size fluctuation might be a concern, since its fluctuation affects the spatial resolution

for inclined tracks. What we need to know is the probability of the primary ionizing collision with an energy transfer "E" to yield "k" 2ndary electrons: $P_2(k; E)$. Once this is known, we can calculate the cluster size distribution as

$$P_{cl}(k) = \int dE \frac{1}{\sigma} \left(\frac{d\sigma}{dE} \right) P_2(k; E)$$

This was done by Lapique and Piuz (1980) for a pure Ar gas. As said above, however, the calculation of $P_2(k; E)$ is a complicated process, since 2ndary ionizing collisions are no longer statistically independent. Their work was hence only partially successful. There is, however, a beautiful measurement by the Heidelberg group (Fischle et al 1991) that can be used in Monte Carlo simulations.

Cluster Size Data

The Heidelberg Group Experiment (Fischle, Heintze, and Schmidt 1991)

Table 2

Cluster size distributions $w(n)$; (a) data points; (b) numerical values referring to the full lines in fig. 12. In brackets extrapolation of the data for $n > n_{\max}$ according to the model described in section 4.3. All numbers in percent.

n	CH ₄		Ar		He		CO ₂	
	(a)	(b)	(a)	(b)	(a)	(b)	(a)	(b)
1	78.7 ± 1.20	78.6	65.6 ± 1.58	65.6	76.7 ± 4.23	76.60	73.0 ± 2.8	72.50
2	11.9 ± 0.35	12.0	14.8 ± 0.67	15.0	11.9 ± 1.46	12.50	16.2 ± 1.2	14.00
3	3.24 ± 0.16	3.4	6.49 ± 0.45	6.4	4.80 ± 0.63	4.60	3.80 ± 0.4	4.20
4	1.34 ± 0.09	1.6	3.37 ± 0.25	3.5	1.61 ± 0.31	2.0	2.00 ± 0.3	2.20
5	0.98 ± 0.09	0.95	2.44 ± 0.19	2.25	0.79 ± 0.26	1.2	1.10 ± 0.20	1.40
6	0.55 ± 0.07	0.60	1.41 ± 0.14	1.55	1.04 ± 0.31	0.75	1.47 ± 0.26	1.00
7	0.57 ± 0.07	0.44	0.78 ± 0.10	1.05	0.63 ± 0.21	0.50	0.60 ± 0.14	0.75
8	0.27 ± 0.05	0.34	0.95 ± 0.11	0.81	0.10 ± 0.09	0.36	0.84 ± 0.19	0.55
9	0.29 ± 0.04	0.27	0.63 ± 0.09	0.61	0.23 ± 0.16	0.25	0.52 ± 0.13	0.46
10	0.20 ± 0.03	0.21	0.62 ± 0.10	0.49	0.15 ± 0.11	0.19	0.20 ± 0.08	0.38
11	0.16 ± 0.03	0.17	0.42 ± 0.08	0.39	0.12 ± 0.11	0.14	0.42 ± 0.14	0.34
12	0.13 ± 0.03	0.13	0.28 ± 0.06	0.30	0.21 ± 0.10	0.10	0.21 ± 0.08	0.28
13	0.10 ± 0.02	0.10	0.18 ± 0.05	0.25	0.37 ± 0.17	0.08	0.25 ± 0.10	0.24
14	0.12 ± 0.02	0.08	0.23 ± 0.07	0.20	0.08 ± 0.07	0.06	0.38 ± 0.13	0.20
15	0.06 ± 0.02	0.06	0.17 ± 0.05	0.16	0.04 ± 0.04	0.048	0.21 ± 0.10	0.16
15		(0.050)	0.14 ± 0.05	0.12	0.00 ± 0.04	(0.043)	0.09 ± 0.06	0.12
17		(0.042)	0.06 ± 0.03	0.095	0.04 ± 0.04	(0.038)	0.13 ± 0.07	0.09
18		(0.037)	0.05 ± 0.02	0.075		(0.034)		(0.064)
19		(0.033)		(0.063)		(0.030)		(0.048)
≥ 20		($w(n) = 11.9/n^2$)		($21.6/n^2$)		($10.9/n^2$)		($14.9/n^2$)

Cluster Size Distribution

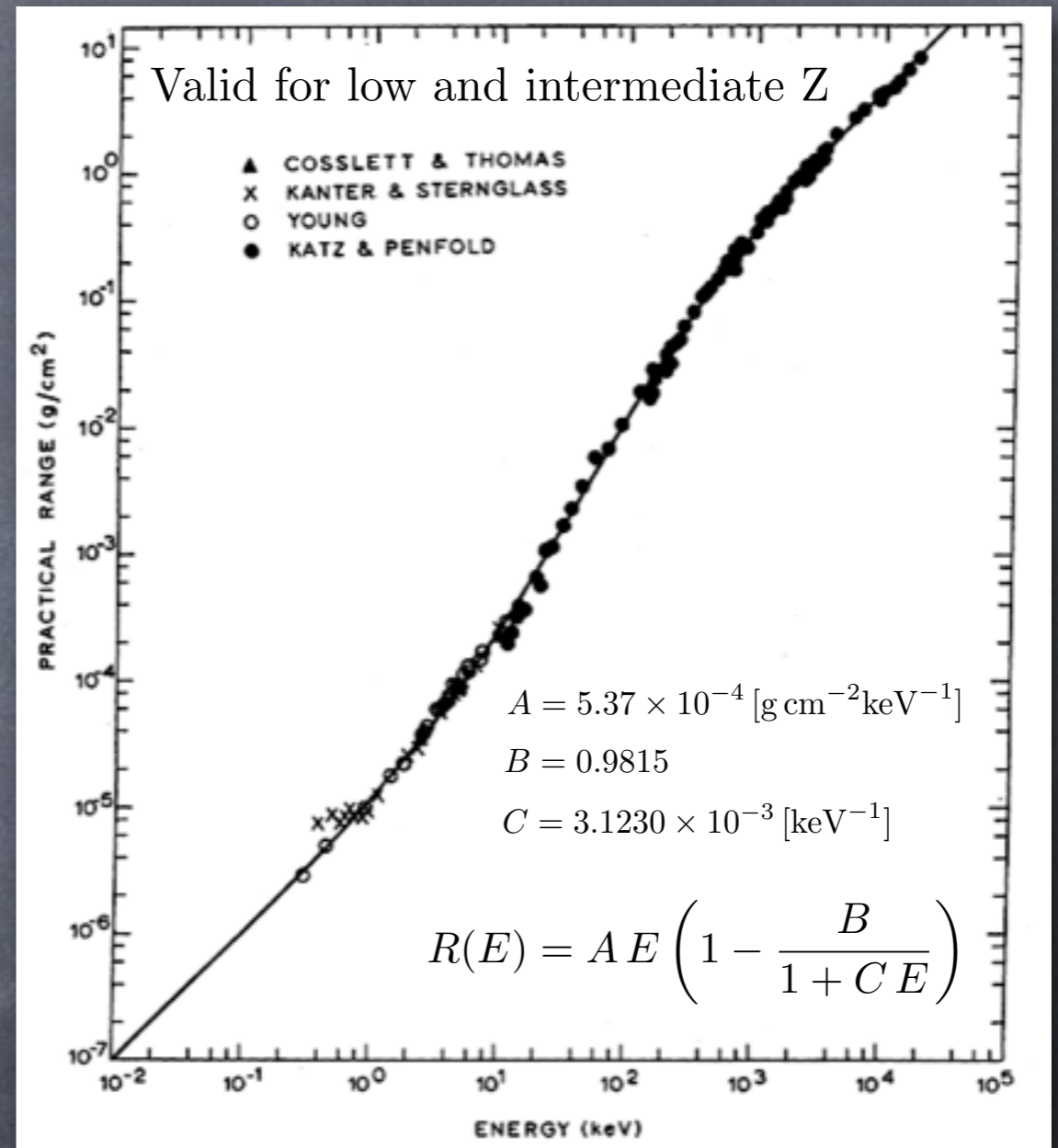
Geometrical Size of Cluster

Geometrical Size

The delta electrons have a finite range and hence give a finite geometrical size to the primary ionization cluster.

Since the electric field due to a relativistic charged particle is perpendicular to its trajectory, the delta electron tends to be kicked out in the perpendicular direction. If the delta ray has a finite range, it would result in a shift of the charge centroid in that direction, deteriorating the spatial resolution. In the case of a TPC operated in a high magnetic field, the delta electron is curled up and hence the transverse cluster size can hardly be affected.

At $B=0$, however, the effect may be visible. I quote here an empirical formula by Kobetich and Katz (1968):



Typical delta-ray range values in Ar (N.T.P.)

$$R(1 [\text{keV}]) \simeq 30 [\mu\text{m}]$$

$$R(10 [\text{keV}]) \simeq 1.5 [\text{mm}] : 0.05 \% \text{ of collisions}$$

Cluster Size Distribution

Appendix (Delta-ray Kinematics)

Kinematics

Let the angle between the incident particle direction and that of the delta-ray emission be ψ , and let the maximum kinetic energy transfer be E_{\max} , we have

$$\cos^2 \psi = \frac{2m_e c^2 + E_{\max}}{2m_e c^2 + E} \frac{E}{E_{\max}}$$

with

$$E_{\max} = \frac{2m_e c^2 \beta^2 \gamma^2}{1 + 2\gamma (m_e/m) + (m_e/m)^2}$$

for a free electron at rest.

This implies that

$$E_{\max} \approx 2m_e c^2 (\beta\gamma)^2 \simeq (\beta\gamma)^2 [\text{MeV}]$$

for a particle with $m \gg m_e$

For a minimum ionizing particle ($\beta\gamma \simeq 4$), we hence have

$$\cos^2 \psi \simeq \frac{E}{2m_e c^2 + E}$$

This formula tells us that on a purely kinematical basis, delta-ray emission should approximately be perpendicular to the incident particle direction, as long as we are talking about a delta-ray with an energy negligible compared to the electron mass.

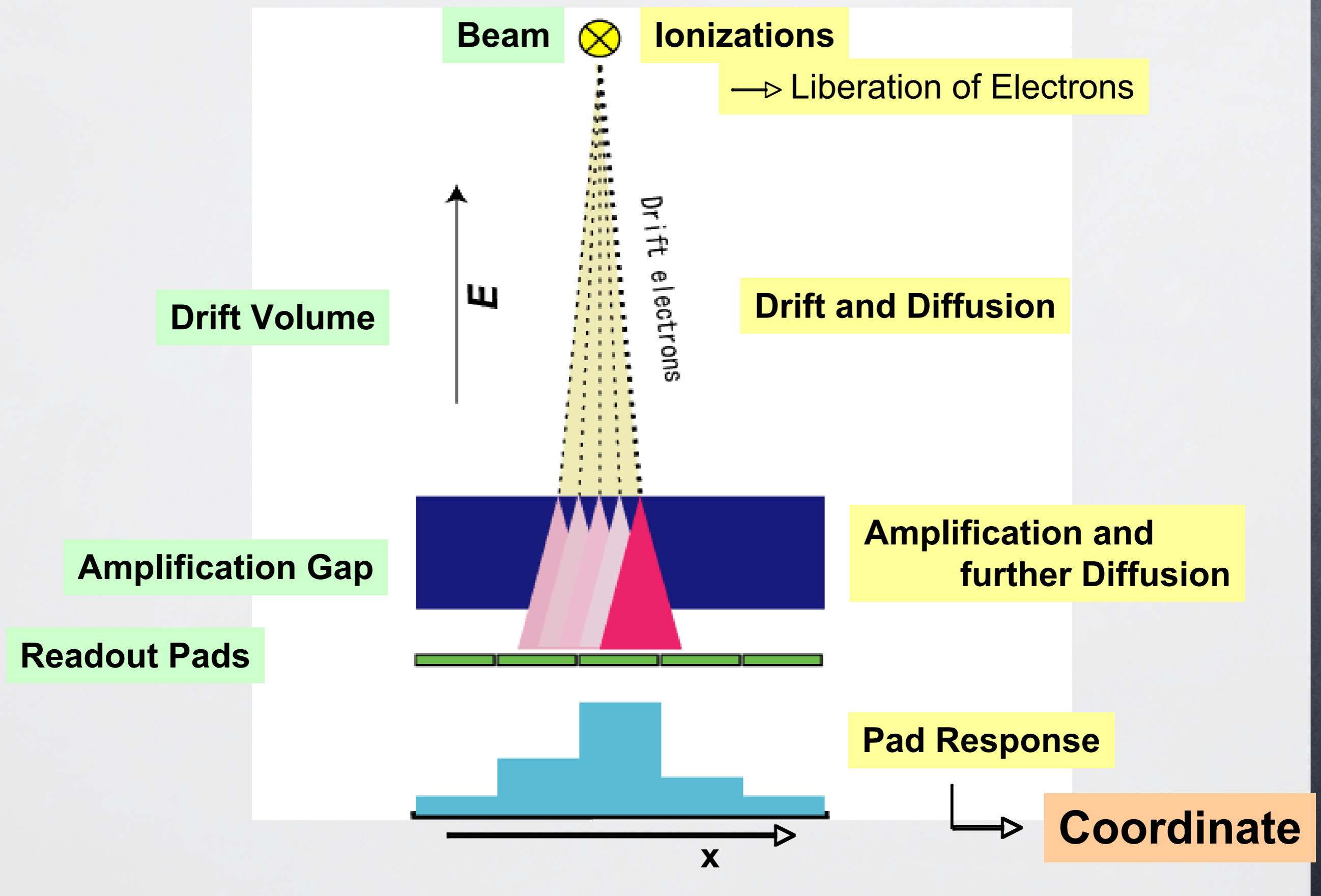


Tracking Detectors

2

Keisuke Fujii, KEK

Fundamental Processes



Classical Theory of Electrons in a Gas

Why Classical Theory?

Is it OK to treat it classically instead of quantum mechanically?

Inter-molecular Distance

$$\begin{aligned} N_A &= 6.02 \times 10^{23} \text{ [mol}^{-1}\text{]} & \longrightarrow & V_1 = (3.3 \text{ [nm]})^3 \text{ per molecule} \\ V &= 2.24 \times 10^4 \text{ [cm}^3\text{/mol]} & & \text{at } 0^\circ\text{C, 1 atm} \\ R_{\text{Ar}} &= 0.18 \text{ [nm]} & & \text{Inter-molecular distance} \\ & & & \simeq 20 \times R_{\text{Ar}} \end{aligned}$$

Thermal Energies

$$\begin{aligned} \left\langle \frac{1}{2} m v^2 \right\rangle &= \left\langle \frac{1}{2} M V^2 \right\rangle = \frac{3}{2} KT = 0.039 \text{ [eV]} & \sqrt{\langle v^2 \rangle} &= 0.39 \times 10^{-3} c \\ \frac{\hbar}{m \sqrt{\langle v^2 \rangle}} &= 0.98 \text{ [nm]} & \sqrt{\langle V^2 \rangle} &= 1.4 \times 10^{-6} c \\ \frac{\hbar}{M_{\text{Ar}} \sqrt{\langle V^2 \rangle}} &= 3.6 \times 10^{-3} \text{ [nm]} & \frac{\sqrt{\langle V^2 \rangle}}{\sqrt{\langle v^2 \rangle}} &\simeq 4 \times 10^{-3} \end{aligned}$$

The de Broglie wave length of the electron is small enough compared to the inter molecular distance implying that it is much smaller than the mean free path. The C.O.G. motion of the electron can hence be treated classically.

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 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

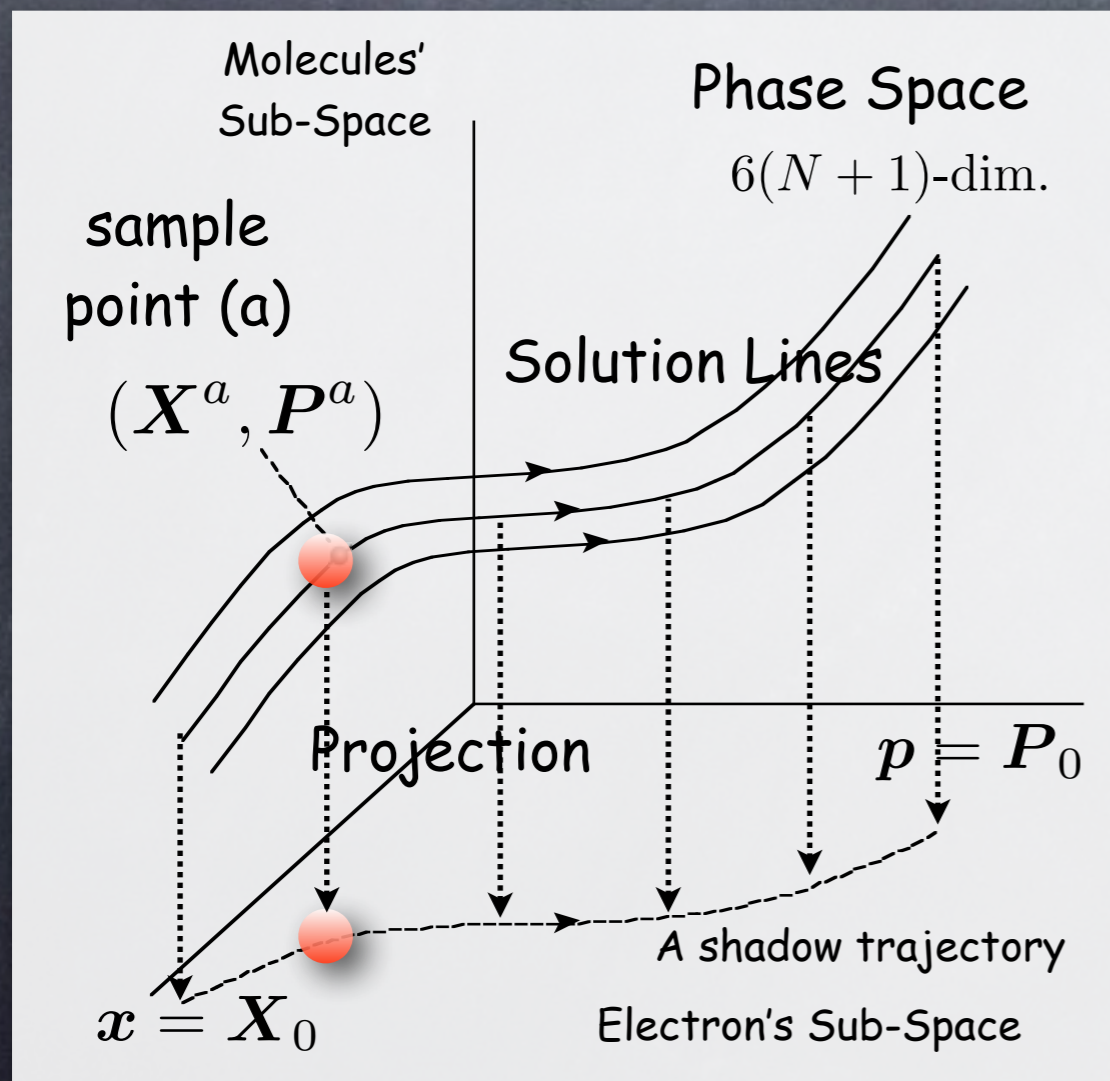
Causal deterministic motion by

$$\begin{aligned}
 H = & \frac{p^2}{2m} + \sum_{b=1}^N \frac{P_b^2}{2M_b} \\
 & + U_{\text{ext}}(\mathbf{x}, \mathbf{p}) && : \text{Lorentz force (E,B)} \\
 & + U_{\text{mM}}(\mathbf{x}, \mathbf{X}) && : \text{elec. + mol. collision} \\
 & + U_{\text{MM}}(\mathbf{X}, \mathbf{X}') && : \text{mol. + mol. collision}
 \end{aligned}$$

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

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

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

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:

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

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

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

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:

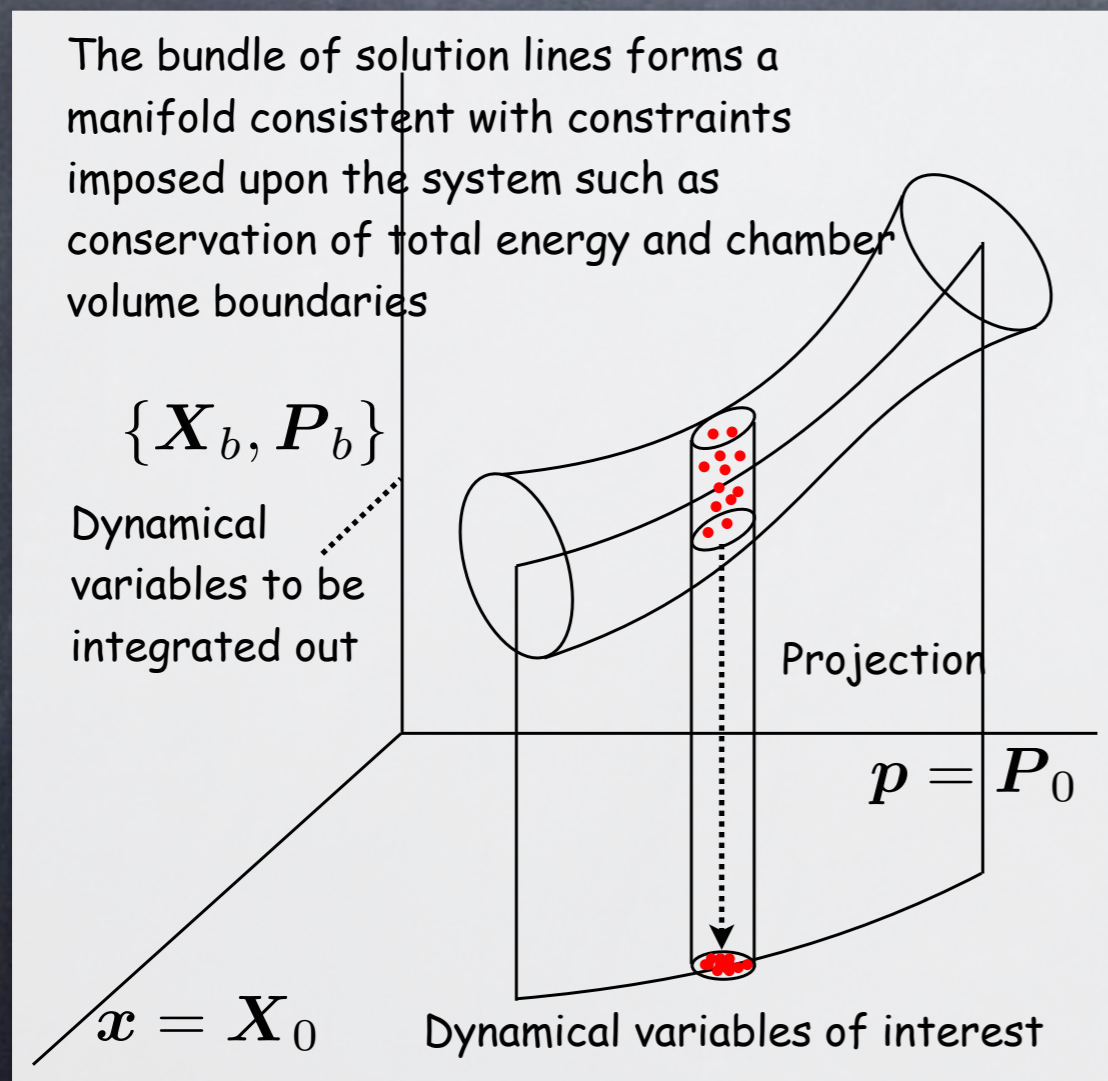
Probability is proportional to phase space volume

Thermal equilibrium = Equal weight

Macroscopic Picture

Projection = Coarsification
= information loss

Projected volume decides probability



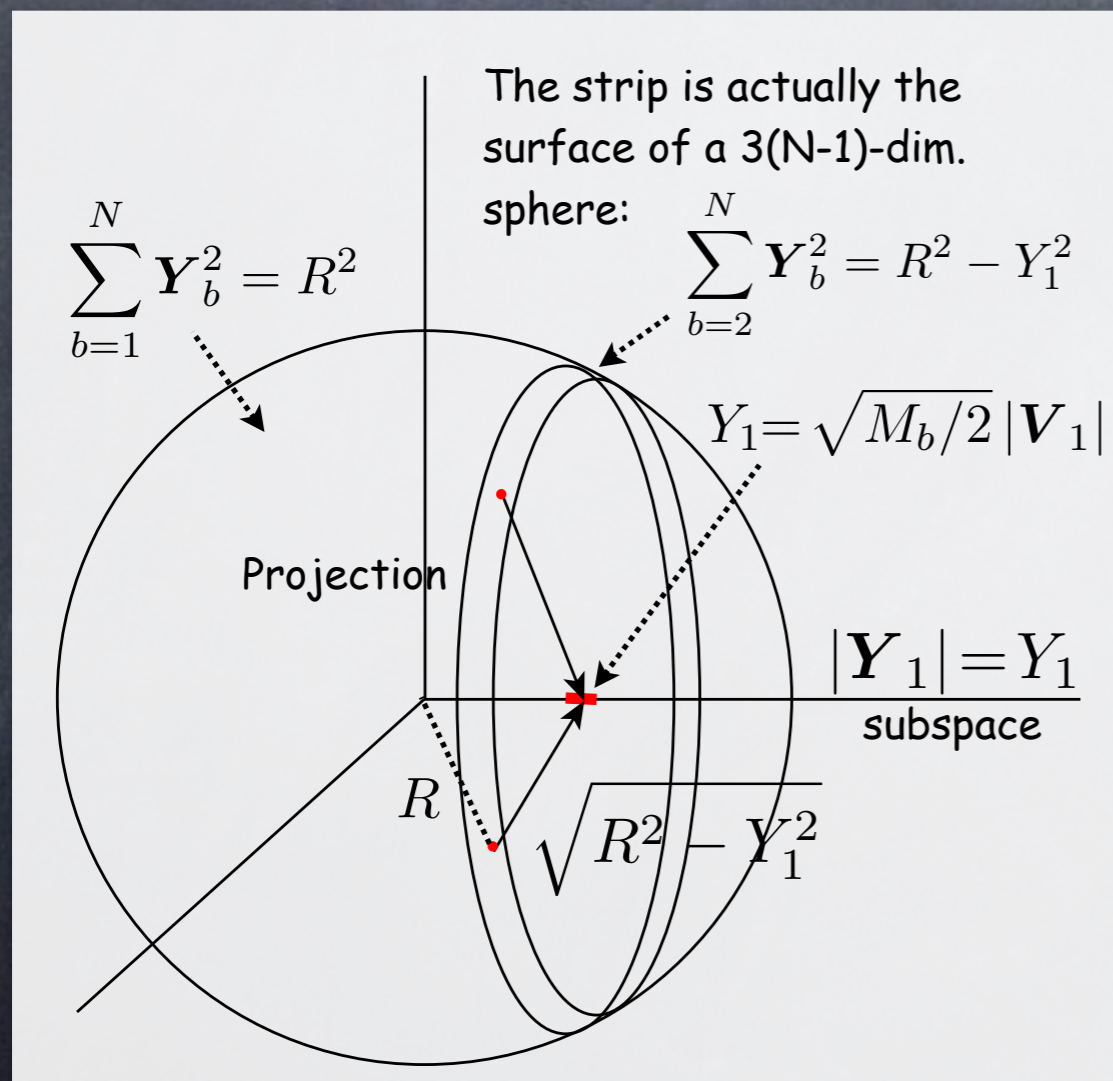
Maxwellian Distribution

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.



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

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

$$S_{3(N-1)} \left(\sqrt{R^2 - Y_1^2} \right)$$

$$\propto \left(\sqrt{R^2 - Y_1^2} \right)^{3(N-1)-1} \approx R^{3N-4} \left[1 - (Y_1/R)^2 \right]^{3N/2}$$

$$\approx R^{3N-4} \left[1 - \frac{Y_1^2 / ((2/3)R^2/N)}{3N/2} \right]^{3N/2}$$

$$\rightarrow R^{3N-4} \exp \left[-\frac{Y_1^2}{(2/3)(R^2/N)} \right] \propto \exp \left[-\frac{Y_1^2}{k_B T} \right]$$

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

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

+ 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:

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

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:

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

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

Then we have

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

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.

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

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.

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

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:

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

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

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

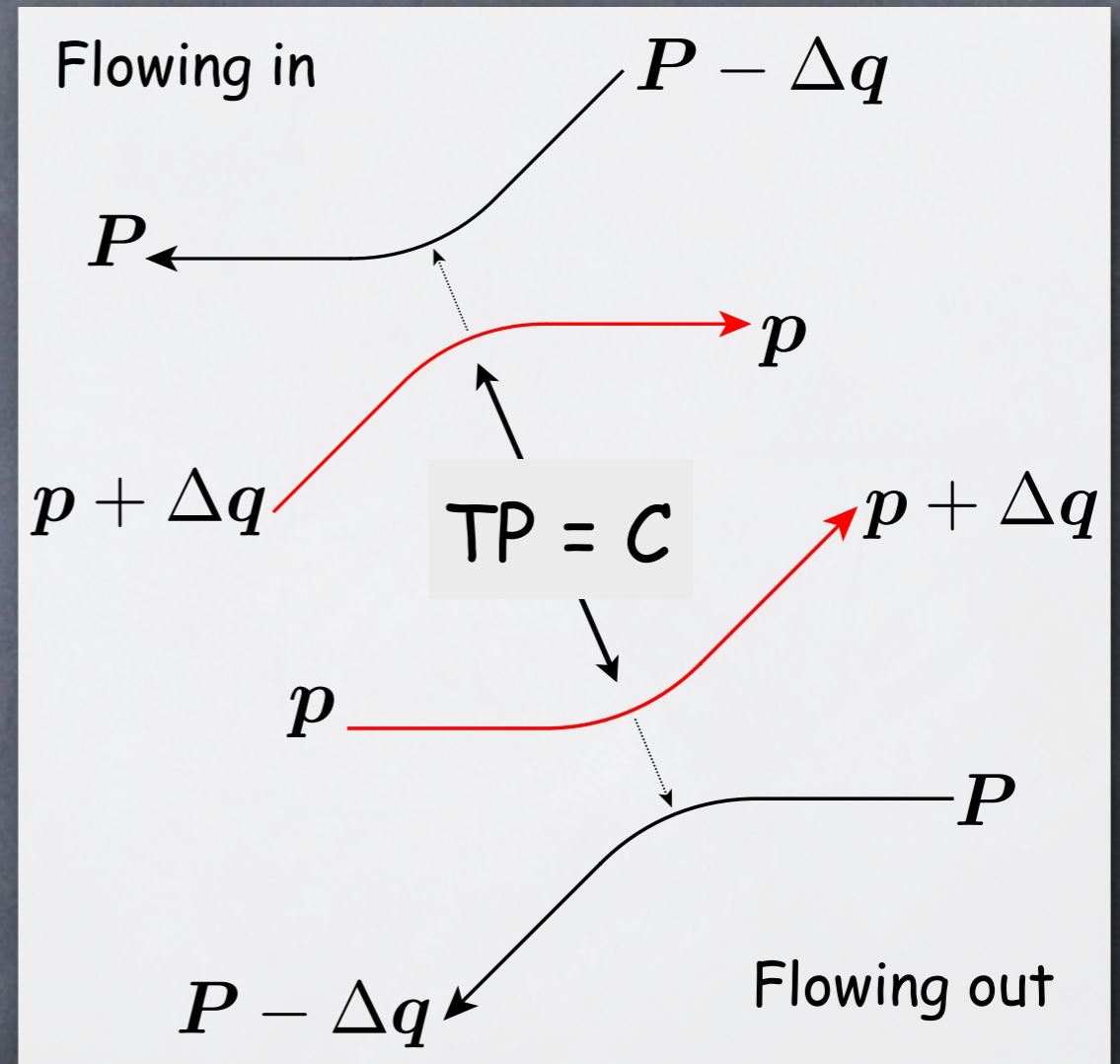
where the external force is given by

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

and the 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 in 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 complicates 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:

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

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

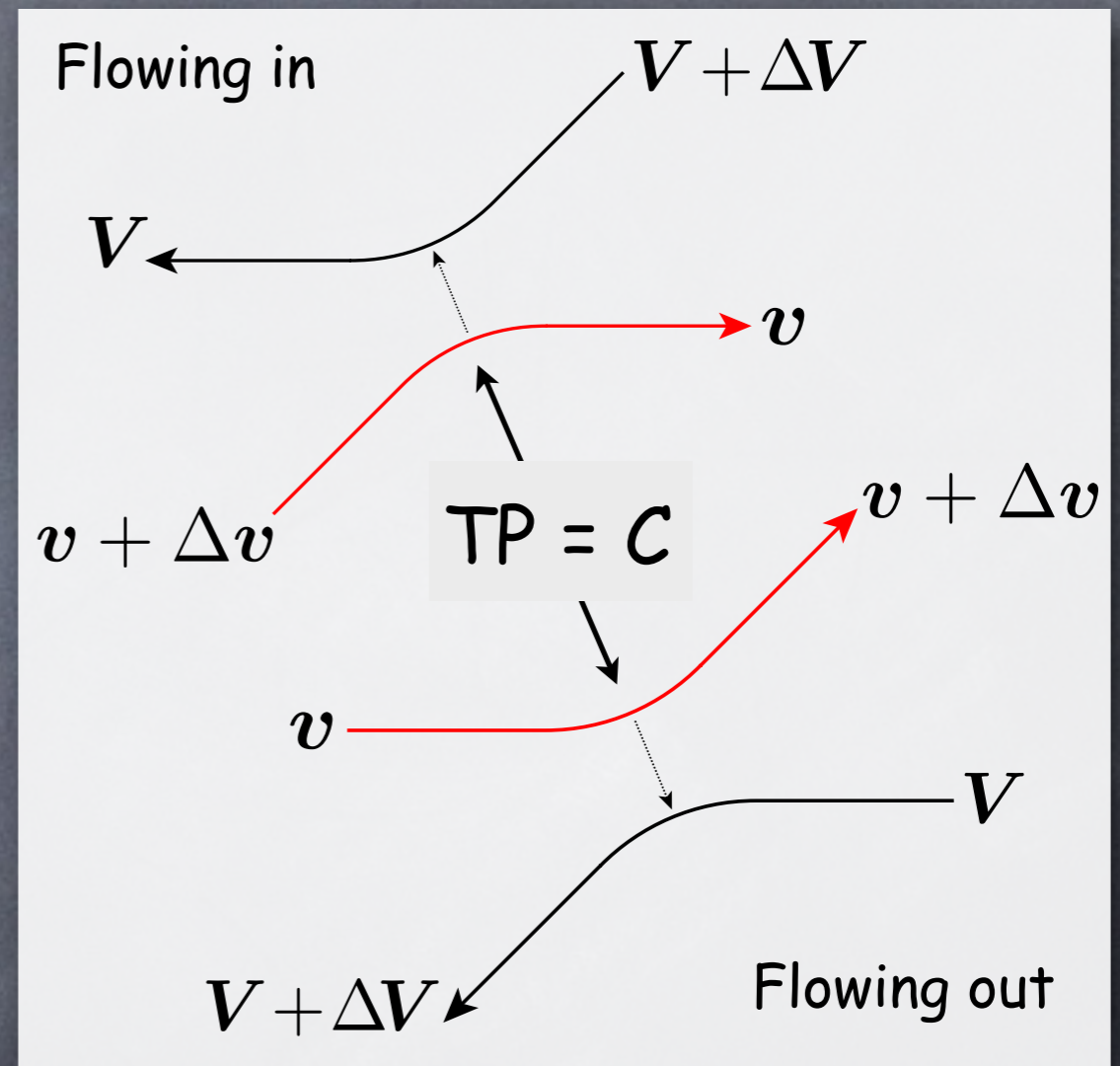
$$\times \left[\underbrace{f(\mathbf{x}, \mathbf{v} + \Delta \mathbf{v}; t)}_{\text{part flowing in}} \bar{F}_k(\mathbf{V} + \Delta \mathbf{V}; t) - \underbrace{f(\mathbf{x}, \mathbf{v}; t)}_{\text{part flowing out}} \bar{F}_k(\mathbf{V}; t) \right]$$

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 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 scaling 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

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

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

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

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

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

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.

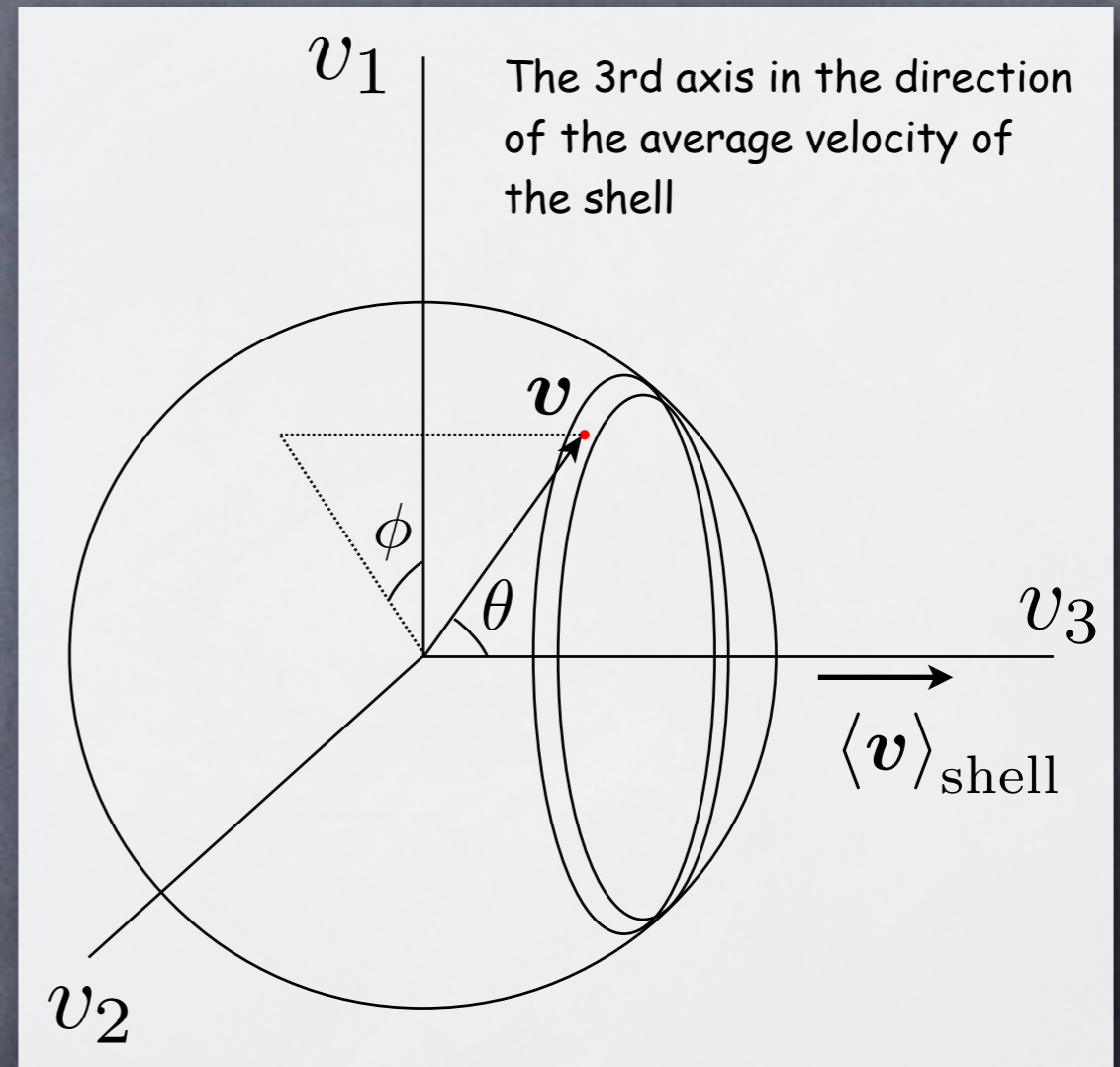
The Basic Idea

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

$$\begin{aligned} \langle \mathbf{v} \rangle_{\Omega_v} &= \int d\Omega_v \mathbf{v} \bar{f}(\mathbf{v}; \mathbf{x}, t) / \int d\Omega_v \bar{f}(\mathbf{v}; \mathbf{x}, t) \\ &= \frac{v}{\sqrt{6} \bar{f}_0^0} \begin{pmatrix} \bar{f}_1^{-1} - \bar{f}_1^1 \\ -i(\bar{f}_1^{-1} + \bar{f}_1^1) \\ \sqrt{2} \bar{f}_1^0 \end{pmatrix} \end{aligned}$$

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

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

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)

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

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

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

Scalar Equation

Interpretation of Scalar Eq.

First recall that the total weight of the velocity shell $(v, v+dv)$ is

$$\tilde{n} dv = (4\pi v^2 dv) (n f_0)$$

while the shell averaged velocity is given by

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

Putting these into the scalar equation

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

and canceling out common factors, we get

net loss of the shell population
due to drift

net gain of the shell population
due to collisions

$$\frac{\partial}{\partial t} \tilde{n} + \frac{\partial}{\partial x} \cdot (\tilde{n} \langle \mathbf{v} \rangle_{\Omega_v}) + \frac{\partial}{\partial v} \left[\frac{e \mathbf{E}}{m} \cdot \frac{\langle \mathbf{v} \rangle_{\Omega_v}}{v} \tilde{n} \right] = \frac{\partial}{\partial v} \left[n \sum_k n_k \bar{\sigma}_{m,k} (v; [f_0]) \right]$$

change rate of the
shell population

net loss of the shell population due heating up due to external fields

The shell population times the $mv^2/2$ is the total energy of the shell, and hence the conservation of population is equivalent to that of energy.

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

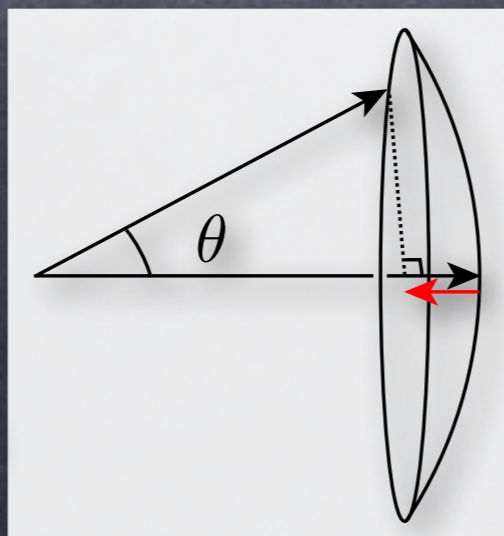
$$\sigma_{m,k} = \sigma_{0,k} - \frac{v'_r}{v_r} \sigma_{1,k}$$

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)

$$\frac{\partial}{\partial t} (n f_1) + v \frac{\partial}{\partial x} (n f_0) + \frac{e \mathbf{E}}{m} \frac{\partial}{\partial v} (n f_0) - \boldsymbol{\omega} \times (n \mathbf{f}_1) = -\bar{v}_m(v) (n \mathbf{f}_1)$$

where

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

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

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

$$d\mathbf{p}_{tot} = (4\pi v^2 dv) (n f_0) m \frac{v \mathbf{f}_1}{3 f_0} = \frac{4\pi v^2 dv}{3} m v (n \mathbf{f}_1)$$

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

$$\tau \frac{\partial}{\partial t} (n \mathbf{f}_1)$$

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

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

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

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

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:

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

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

Notice that these are linear equations of the form

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

that can be solved by matrix inversion,

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

once f_0 is given.

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

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

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

$$\begin{aligned} \langle \mathbf{v} \rangle &= \int d^3 \mathbf{x} \int (4\pi) v^2 dv (n f_0) \mathbf{W} \\ &= \int \left(\frac{4\pi}{3} \right) v^3 dv \int d^3 \mathbf{x} (n \mathbf{f}_1) \end{aligned}$$

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 fE , which can be rewritten with WE 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 $[M]$:

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

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 M is given by

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

with

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

and

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

WE can now be written as

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

which can be averaged over v to give

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

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

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

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 appear the mean free time and the average momentum transfer.

The momentum transfer averaged over all angles is easy to get for isotropic collisions

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

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 v distribution or of a single velocity shell. We can also rewrite the Langevin equation in the following form

$$[1 - \omega\tau \times] \langle \mathbf{v} \rangle = \frac{e\tau}{m} \mathbf{E} \quad \mu(B=0)$$

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**.

The Inverse of [M]

Another Expression

The drift velocity formula for a single shell

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

can be rewritten as

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

This implies that the inverse of [M] can be cast into the form

$$[M]^{-1} = \left(\frac{\tau}{1 + (\omega\tau)^2} \right) \left[1 + (\omega\tau) \hat{\mathbf{B}} \times + (\omega\tau)^2 \hat{\mathbf{B}} \hat{\mathbf{B}} \cdot \right]$$

From this we have immediately

$$\hat{\mathbf{B}}^T [M]^{-1} \hat{\mathbf{B}} = \tau$$

and

$$\hat{\mathbf{e}}_{\perp}^T [M]^{-1} \hat{\mathbf{e}}_{\perp} = \frac{\tau}{1 + (\omega\tau)^2}$$

where $\hat{\mathbf{e}}_{\perp}$ is a unit vector perpendicular to the B-field. We will see later that the

diffusion matrix is given by

$$[D] = \frac{1}{3} \left\langle v^2 [M]^{-1} \right\rangle$$

Twice integrating by parts the diffusion eq. in the comoving frame, we have

$$\begin{aligned} \frac{d}{dt} \int d^3 \mathbf{x}' n(\mathbf{x}'; t) (\mathbf{x}' \cdot \mathbf{e})^2 &= \int d^3 \mathbf{x}' \left(\frac{\partial}{\partial \mathbf{x}'} \right)^T \frac{1}{3} \left\langle v^2 [M]^{-1} \right\rangle \left(\frac{\partial}{\partial \mathbf{x}'} \right) n(\mathbf{x}'; t) (\mathbf{x}' \cdot \mathbf{e})^2 \\ &= \int d^3 \mathbf{x}' \frac{2}{3} \left\langle v^2 \mathbf{e}^T [M]^{-1} \mathbf{e} \right\rangle n(\mathbf{x}'; t) \\ &= \frac{2}{3} \left\langle v^2 \mathbf{e}^T [M]^{-1} \mathbf{e} \right\rangle \end{aligned}$$

This implies

$$\frac{d}{dt} \sigma_{x_e}^2 = 2D_e = \frac{2}{3} \left\langle v^2 \mathbf{e}^T [M]^{-1} \mathbf{e} \right\rangle$$

and hence

$$D_L = \frac{1}{3} \left\langle v^2 \tau \right\rangle \quad \text{and} \quad D_T = \frac{1}{3} \left\langle v^2 \frac{\tau}{1 + (\omega\tau)^2} \right\rangle$$

Diffusion

Diffusion Matrix

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:

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

Notice that this time, since $n(\mathbf{x};t)$ depends on \mathbf{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

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

and

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

The solution is then

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

which can be averaged over v to give

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

Diffusion

Diffusion Matrix (Continued)

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:

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

with

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

and

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

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

$$\underbrace{n \langle \mathbf{W}_G \rangle_v}_{\text{current density (w/o common drift)}} = - [D] \underbrace{\frac{\partial}{\partial \mathbf{x}} n}_{\text{grad (density)}}$$

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

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

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

Random Walk

Diffusion Matrix (continued)

Usual Simplistic Arguments

Case (3) formula is usually obtained by the random walk theory with a fixed mean free time:

$$\bar{\tau} = \frac{1}{\nu(\bar{v})}$$

The probability for the electron to fly over a time "t" and then get scattered by the molecule by an angle "Omega" is given by

$$P(t, \Omega) = \frac{1}{\bar{\tau}} \exp\left[-\frac{t}{\bar{\tau}}\right] dt \frac{d\Omega}{4\pi}$$

if the scattering is isotropic. For the sake of simplicity, let us further assume that there is no E and B along the 3rd axis, then Newton's eq. reads

$$\frac{d}{dt} \mathbf{v} = \boldsymbol{\omega} \times \mathbf{v}$$

The solution to this is a helix

$$\mathbf{x}(t) = \frac{\bar{v}}{\omega} \begin{pmatrix} \sin \theta (\cos(\omega t + \phi) - \cos \phi) \\ \sin \theta (\sin(\omega t + \phi) - \sin \phi) \\ \omega t \cos \theta \end{pmatrix} + \mathbf{x}_0$$

If we have N collisions over the time t, the probability of finding the electron at x is

$$P(\mathbf{x}) = \prod_{i=1}^N \left(\int_0^\infty dt_i \frac{1}{\bar{\tau}} e^{-t_i/\bar{\tau}} \int \frac{d\Omega_i}{4\pi} \right) \times \delta^3 \left(\mathbf{x} - \sum_{i=1}^N \Delta \mathbf{x}(\theta_i, \phi_i, t_i) \right)$$

with

$$\Delta \mathbf{x} = \mathbf{x} - \mathbf{x}_0$$

The average position is apparently zero because of the angular integrals which are isotropic.

$$\langle \mathbf{x} \rangle = \int d^3 \mathbf{x} P(\mathbf{x}) \mathbf{x} = \mathbf{0}$$

Random Walk

Diffusion Matrix (continued)

Now the mean square transverse distance is given by

$$\begin{aligned}\sigma_{\perp}^2 &= \sigma_{x_1}^2 + \sigma_{x_2}^2 = \int d^3 \mathbf{x} P(\mathbf{x}) (x_1^2 + x_2^2) \\ &= \left(\frac{\bar{v}}{\omega}\right)^2 \prod_{i=1}^N \left(\int_0^{\infty} dt_i \frac{1}{\bar{\tau}} e^{-t_i/\bar{\tau}} \int \frac{d\Omega_i}{4\pi} \right) \\ &\quad \times \sum_{i=1}^N 2 \sin^2 \theta_i (1 - \cos(\omega t_i)) \\ &= N \left(\frac{\bar{v}}{\omega}\right)^2 \int_0^{\infty} dt' \frac{1}{\bar{\tau}} e^{-t'/\bar{\tau}} \int \frac{d\Omega}{4\pi} 2 \sin^2 \theta (1 - \cos(\omega t')) \\ &= \frac{t}{\bar{\tau}} \left(\frac{\bar{v}}{\omega}\right)^2 \int_0^{\infty} dt' \frac{1}{\bar{\tau}} e^{-t'/\bar{\tau}} \frac{4}{3} (1 - \cos(\omega t')) \\ &= t \frac{4}{3} \frac{(\bar{v}\bar{\tau})^2}{\bar{\tau} (1 + (\omega\bar{\tau})^2)} = 2 \sigma_T^2 = 2 \cdot 2 D_T t\end{aligned}$$

which leads us to the expression

$$D_T = \frac{1}{3} \frac{(\bar{v}\bar{\tau})^2}{\bar{\tau} (1 + (\omega\bar{\tau})^2)}$$

Similarly the mean square longitudinal distance is given by

$$\begin{aligned}\sigma_L^2 &= \sigma_{x_3}^2 = \int d^3 \mathbf{x} P(\mathbf{x}) x_3^2 \\ &= \bar{v}^2 \prod_{i=1}^N \left(\int_0^{\infty} dt_i \frac{1}{\bar{\tau}} e^{-t_i/\bar{\tau}} \int \frac{d\Omega_i}{4\pi} \right) \sum_{i=1}^N t_i^2 \cos^2 \theta_i \\ &= N \bar{v}^2 \int_0^{\infty} dt' \frac{1}{\bar{\tau}} e^{-t'/\bar{\tau}} \int \frac{d\Omega}{4\pi} t'^2 \cos^2 \theta \\ &= \frac{t}{\bar{\tau}} \bar{v}^2 \int_0^{\infty} dt' \frac{1}{\bar{\tau}} e^{-t'/\bar{\tau}} \frac{1}{3} t'^2 \\ &= t \frac{2}{3} \frac{(\bar{v}\bar{\tau})^2}{\bar{\tau}} = 2 D_L t\end{aligned}$$

yielding

$$D_L = \frac{1}{3} \frac{(\bar{v}\bar{\tau})^2}{\bar{\tau}}$$

We reencounter the familiar result

$$\frac{D_T}{D_L} = \frac{1}{1 + (\omega\bar{\tau})^2}$$

Diffusion

Diffusion Matrix (continued)

Case [2] (B//E) Revisited

Now go back to B//E, and rewrite the diffusion constants

$$D_T = \frac{1}{3} \int dv \frac{(4\pi v^2) f_0^*(v) \tau(v)}{1 + (\omega\tau(v))^2} v^2$$

It is interesting to consider the following two extreme cases:

(a) $\omega\tau \ll 1$

$$\begin{aligned} D_T(B) &\approx \frac{1}{3} \int dv (4\pi v^2) f_0^*(v) \tau(v) \\ &\quad \times \left[1 - (\omega\tau(v))^2 \right] v^2 \\ &= \frac{1}{3} \left[\langle \tau v^2 \rangle - \omega^2 \langle \tau^3 v^2 \rangle \right] \\ &\approx \frac{1}{3} \frac{\langle \tau v^2 \rangle}{1 + \omega^2 \langle \tau^3 v^2 \rangle / \langle \tau v^2 \rangle} \\ &= \frac{D_T(0)}{1 + \omega^2 \langle \tau^3 v^2 \rangle / \langle \tau v^2 \rangle} \end{aligned}$$

This implies

$$\frac{D_T(0)}{D_T(B)} \approx 1 + (\omega\tau_1)^2 \quad \text{with} \quad \tau_1^2 = \frac{\langle \tau^3 v^2 \rangle}{\langle \tau v^2 \rangle}$$

valid for a low B-field.

(b) $\omega\tau \gg 1$

$$\begin{aligned} D_T(B) &\approx \frac{1}{3} \int dv (4\pi v^2) f_0^*(v) \tau(v) \\ &\quad \times \left[(\omega\tau(v))^{-2} - (\omega\tau(v))^{-4} \right] v^2 \\ &= \frac{1}{3} \left[\left\langle \frac{v^2}{\omega^2 \tau} \right\rangle - \left\langle \frac{v^2}{\omega^4 \tau^3} \right\rangle \right] \\ &\approx \frac{1}{3} \frac{\langle \tau v^2 \rangle}{\langle \tau v^2 \rangle \langle \frac{v^2}{\tau^3} \rangle / \langle \frac{v^2}{\tau} \rangle^2 + \omega^2 \langle \tau v^2 \rangle \langle \frac{v^2}{\tau} \rangle / \langle \frac{v^2}{\tau} \rangle^2} \\ &= \frac{D_T(0)}{\langle \tau v^2 \rangle \langle \frac{v^2}{\tau^3} \rangle / \langle \frac{v^2}{\tau} \rangle^2 + \omega^2 \langle \tau v^2 \rangle \langle \frac{v^2}{\tau} \rangle / \langle \frac{v^2}{\tau} \rangle^2} \end{aligned}$$

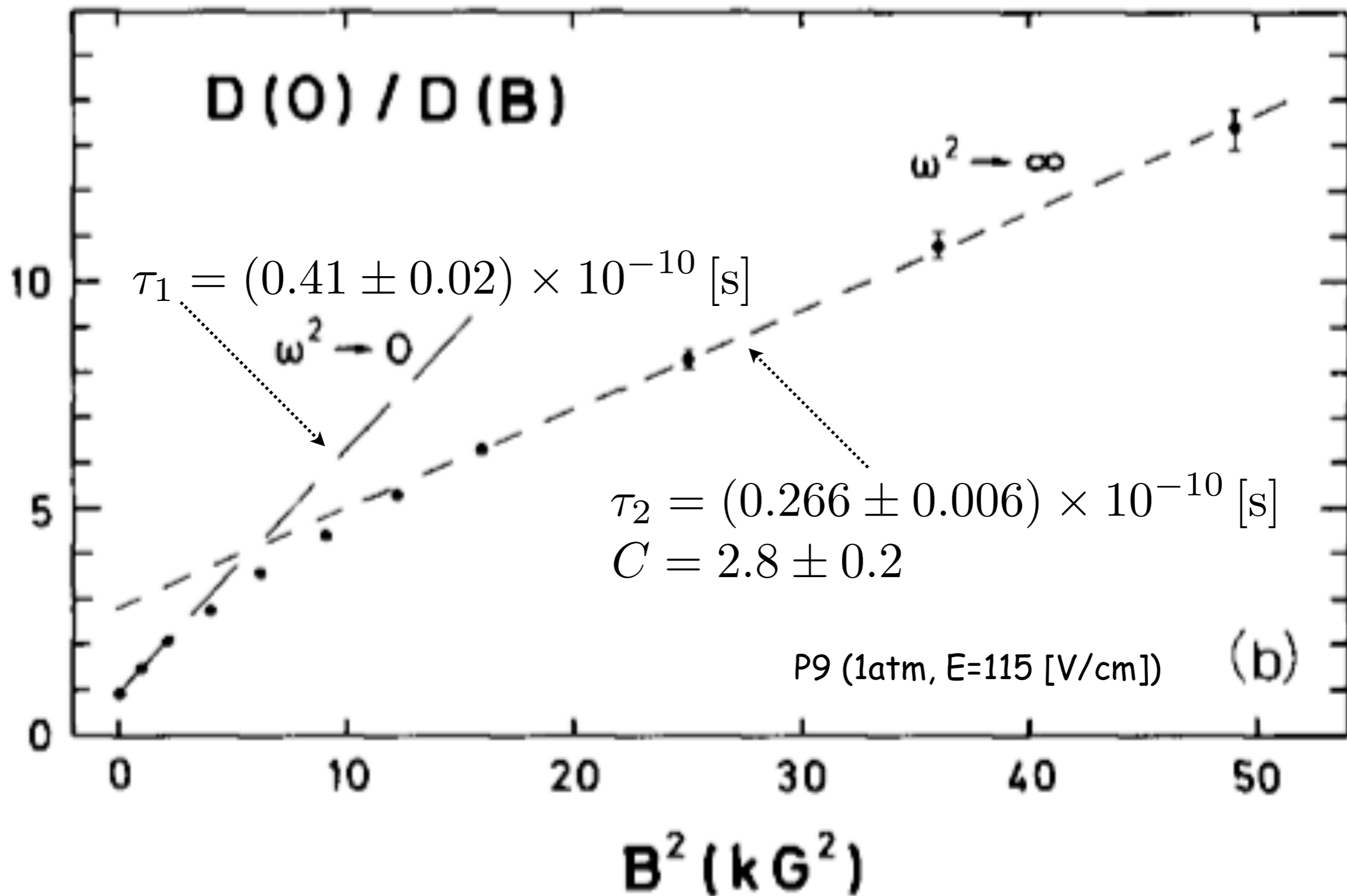
This implies

$$\frac{D_T(0)}{D_T(B)} \approx C + (\omega\tau_2)^2$$

with

$$C = \frac{\langle \tau v^2 \rangle \langle \frac{v^2}{\tau^3} \rangle}{\langle \frac{v^2}{\tau} \rangle^2} \quad \text{and} \quad \tau_2^2 = \frac{\langle \tau v^2 \rangle \langle \frac{v^2}{\tau} \rangle}{\langle \frac{v^2}{\tau} \rangle^2}$$

valid for a high B-field.



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 restart 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

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

with

$$u := \frac{e E}{m v} = \frac{e E}{m} \tau$$

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

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

with

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

has the solution

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

Once the momentum transfer X-section is known, $\nu(v)$ is known, and hence we can calculate f_0^* . That's the recipe.

Special Case I ($E=0$)

In this case $u=0$, and since

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

we end up with

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

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 is 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 an 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 $n=3$.

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

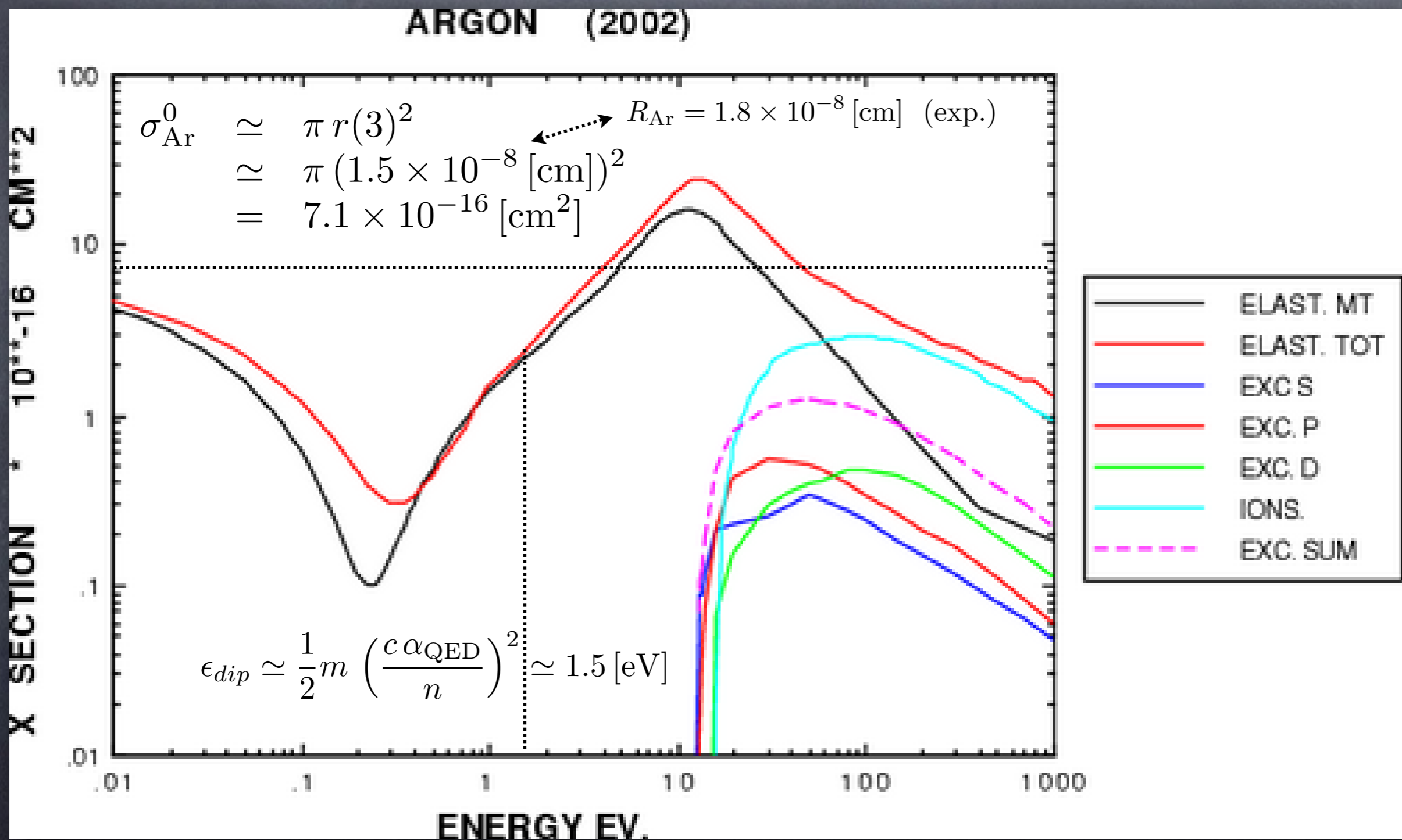
But the life is not so simple, This gives a kind of upper limit, and the real X-section can be much smaller because of the so called Ramsauer effect, a QM effect.

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

The interference makes a dip below the resonance peak!

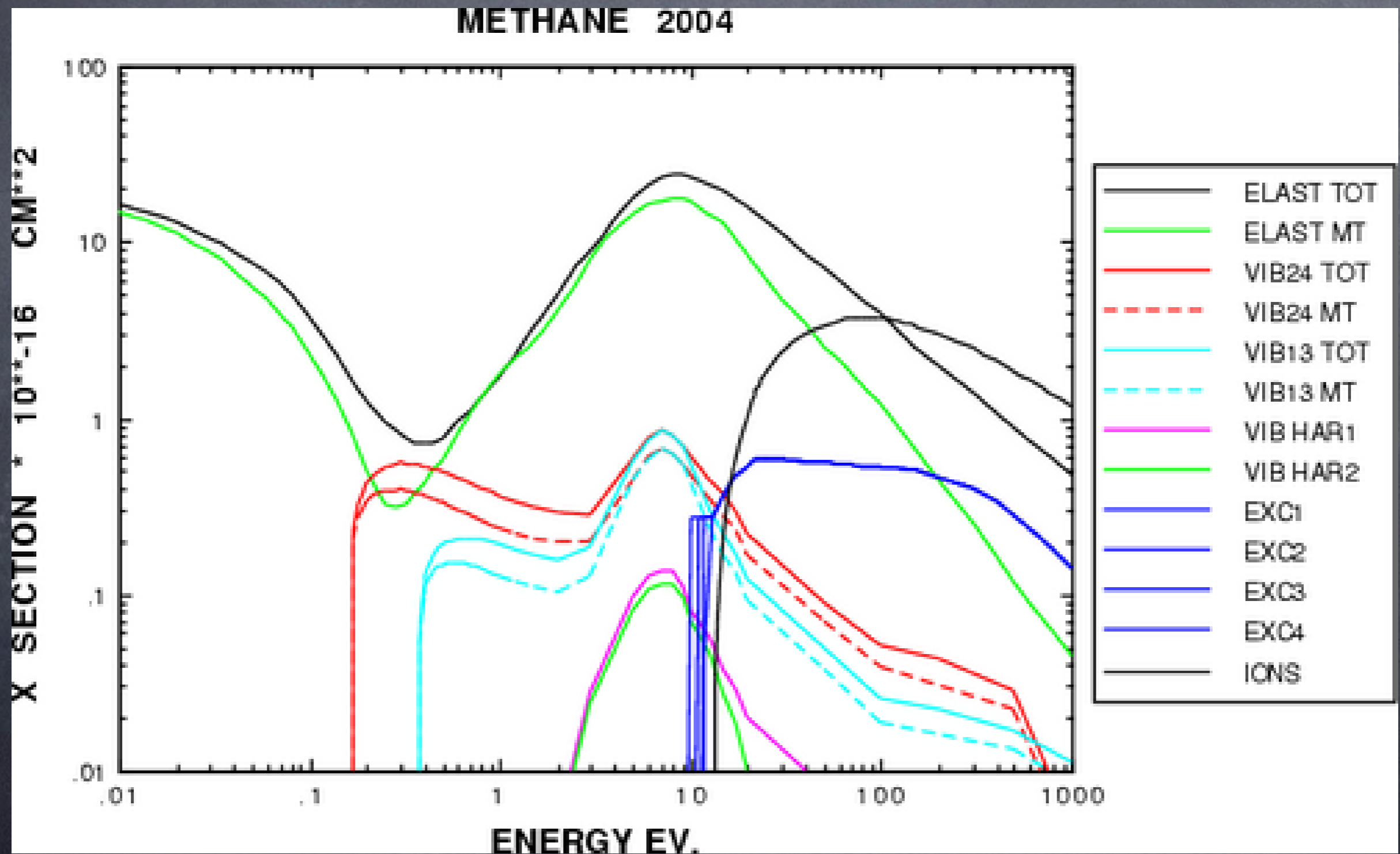
Ar Cross Section

That used in Magboltz



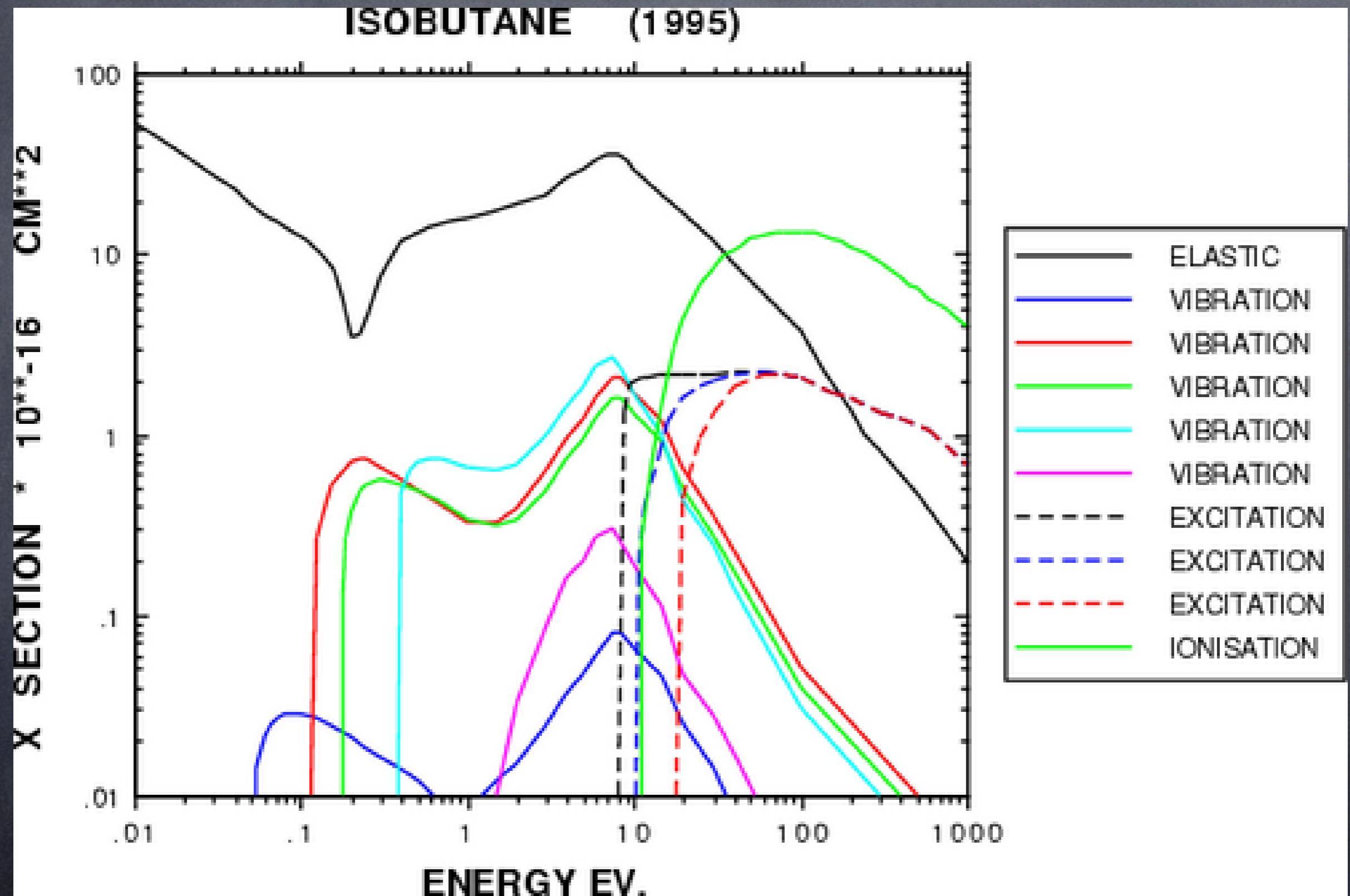
CH4 Cross Section

That used in Magboltz



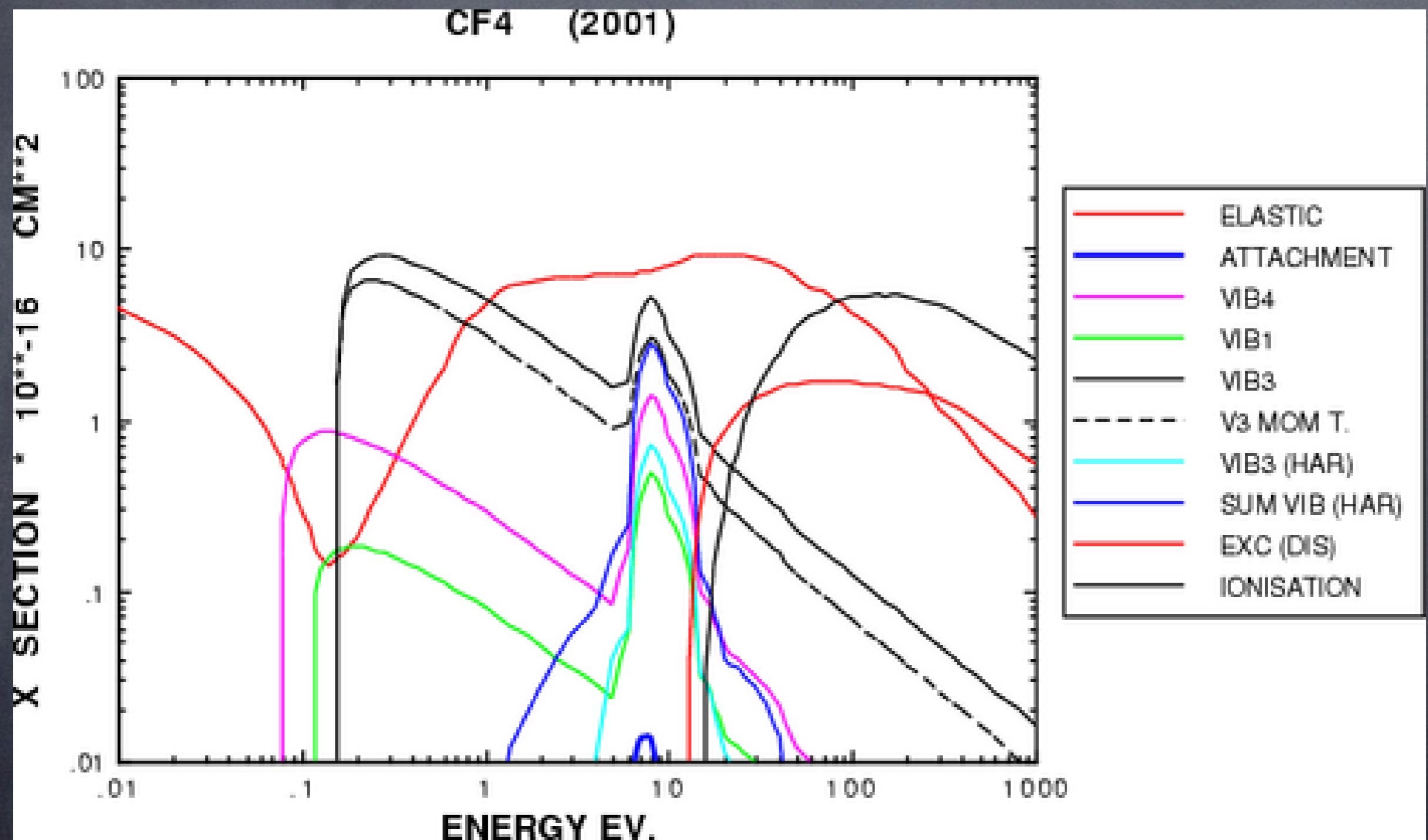
C4H10 Cross Section

That used in Magboltz



CF4 Cross Section

That used in Magboltz



Characteristic Energy

Mobility and Momentum Transfer Cross Section

For simplicity, we will assume $B=0$ here. In this case the mobility constant can be cast into the form

$$\begin{aligned}\mu^* &= -\frac{4\pi e}{3m} \int_0^\infty dv v^3 \tau(v) \left(\frac{d}{dv} f_0^*(v) \right) \\ &= -\frac{4\pi e}{3m} \int_0^\infty dv \left[\left(\frac{d}{dv} v^3 \tau(v) f_0^*(v) \right) - \frac{d}{dv} (v^3 \tau(v)) f_0^*(v) \right] \\ &= \frac{4\pi e}{3m} \int_0^\infty dv \frac{d}{dv} (v^3 \tau(v)) f_0^*(v) \\ &= \frac{4\pi e}{3m} \int_0^\infty dv v^2 \left[3\tau(v) + v \left(\frac{d}{dv} \tau(v) \right) \right] f_0^*(v) \\ &= \frac{e}{m} \langle \tau \rangle + \frac{e}{3m} \left\langle v \frac{d}{dv} \tau \right\rangle\end{aligned}$$

where use has been made of the fact that f_0^* vanishes at the boundaries. If τ is constant, we recover our simple-minded formula. The μ^* becomes max. with τ .

We can further rewrite the formula as

$$\mu = \frac{2e}{3m} \langle \tau \rangle + \frac{e}{3m} \left\langle \frac{d}{dv} (v\tau) \right\rangle$$

Here we used a shorthand, $\mu^* = \mu$, since there is no fear for confusion.

Recalling that $(v\tau)$ is inverse of the gas density times the effective momentum transfer X-section, the 2nd term vanishes if the X-section change is negligible over the velocity distribution given by f_0^* . This is true near the X-section minimum. On the falling edge it is +ve and on the rising edge it is -ve.

On the other hand, (roughly speaking) the 1st term attains its maximum near the X-section minimum. Net effect is that the mobility attains its maximum near the Ramsauer dip.

Characteristic Energy

eD/μ as an estimate of the average electron energy

Characteristic Energy

The diffusion constant at $B=0$ is given by

$$D = \frac{1}{3} \int_0^\infty dv (4\pi v^2) f_0^*(v) (v^2 \tau(v)) = \frac{1}{3} \langle v^2 \tau \rangle$$

which can be cast into the form

$$D = \frac{2}{3m} \left\langle \frac{1}{2} m v^2 \tau \right\rangle$$

Recalling

$$\mu = \frac{e}{m} \langle \tau \rangle + \frac{e}{3m} \left\langle v \frac{d}{dv} \tau \right\rangle$$

and ignoring the variation of τ over the velocity range determined by f_0^* , we have

$$\epsilon_k := \frac{eD}{\mu} \approx \frac{2}{3} \left\langle \frac{1}{2} m v^2 \right\rangle$$

The quantity (eD/μ) is termed the characteristic energy of the electron for obvious reason.

Nernst-Townsend Formula

In the thermal limit, the characteristic energy is given by

$$\frac{D e}{\mu} = k_B T = 0.025 \text{ [eV]} \quad (1 \text{ atm, } 20^\circ \text{C})$$

and called the Nernst-Townsend formula. For a cool gas such as CO_2 , this formula holds up to about 1 kV/cm , while for Ar , this breaks down at an E -field value as low as 1 V/cm . The electrons in a pure Ar gas can be easily heated up to 1 eV or higher.

In the thermal limit, C_d (the diffusion coefficient: the rms size of a cluster after a unit length of drift) is given by

$$C_d := \sqrt{\frac{2D}{\mu E}} \approx \sqrt{\frac{2k_B T}{E}}$$

Cd and Vd for CO2

Trying to understand Magboltz results (B//E)

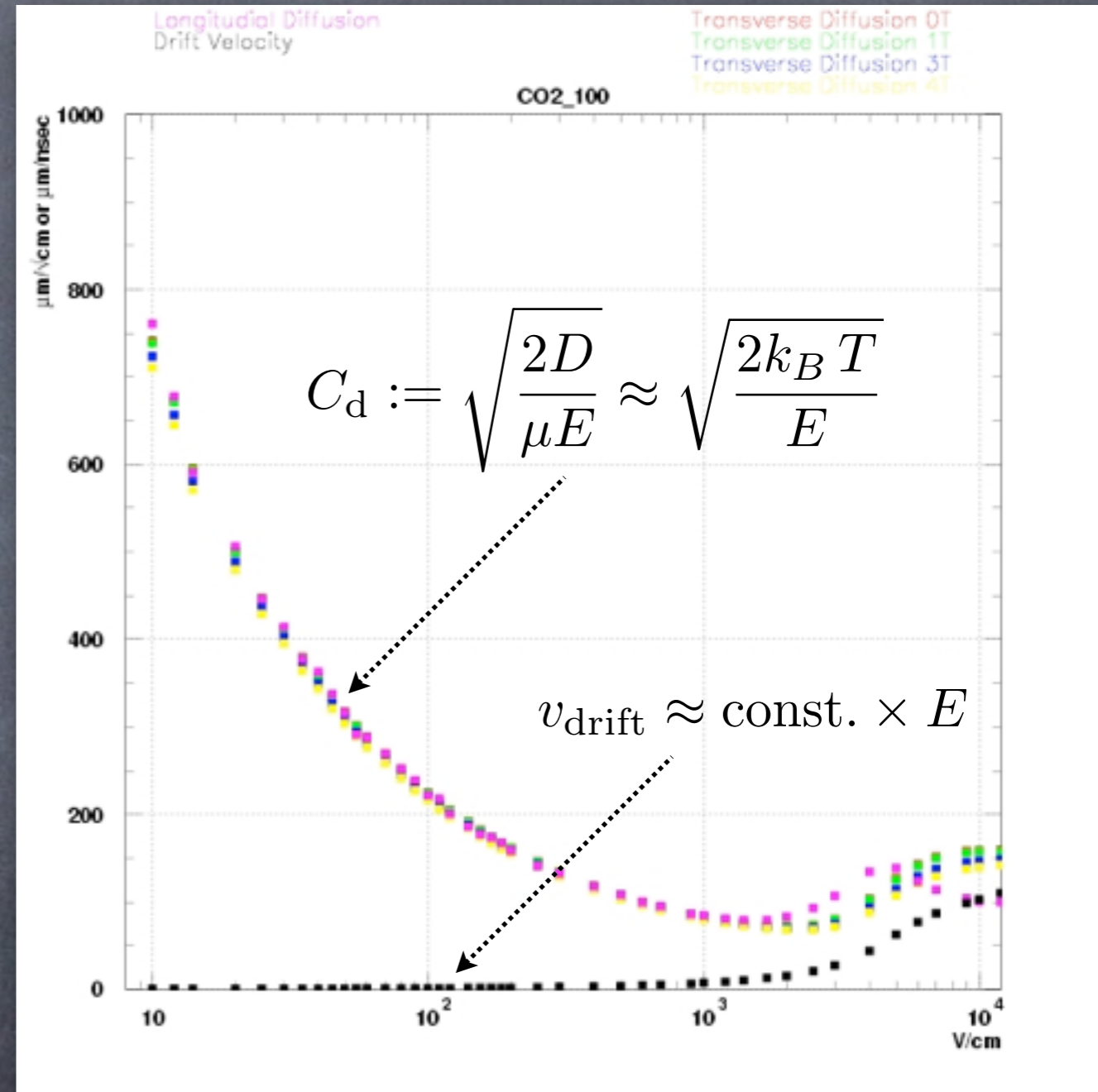
It is interesting to test the expectation with the simulation by Magboltz.

We can see that the diffusion coefficient C_d behaves as $1/\sqrt{E}$ up to 1kV/cm with almost no dependence on the B-field.

The almost no dependence of C_d on B can be understood as the consequence of the smallness of ωT .

It is also worth noting that the mobility is approximately constant and hence the drift velocity is proportional to the E-field in the same region: $E < 1\text{kV/cm}$.

The fact that the electron velocity stays thermal up to rather high E-fields is attributable to many excitation modes of CO2 to cool the electrons.



Cd and Vd for P5

Trying to understand Magboltz results (B//E)

In the case of P5, a more suitable gas for a TPC, the behavior is very different.

First notice the strong dependence of the diffusion constant on the B-field, which suggests

$$\omega\tau \gg 1$$

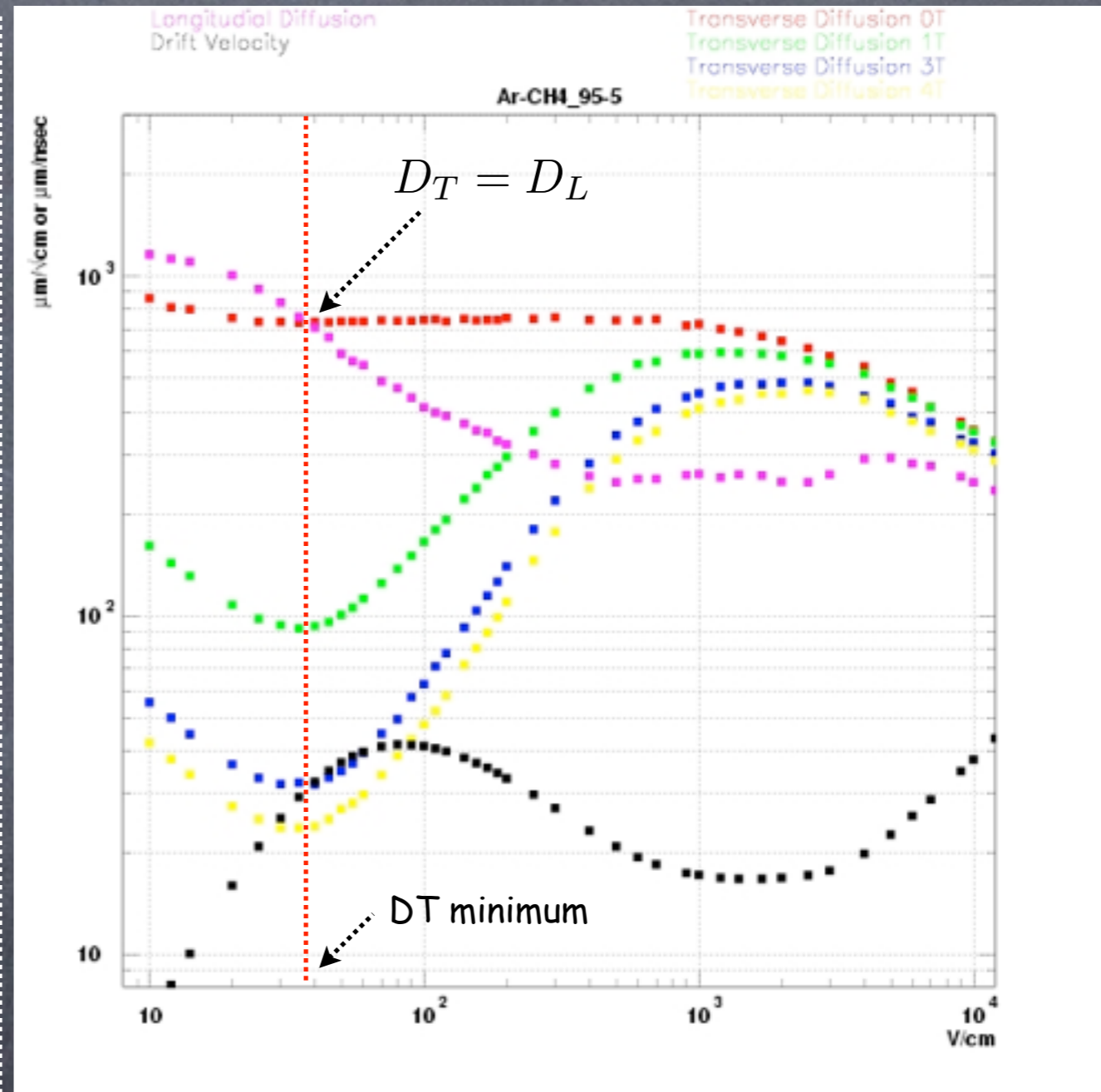
and hence

$$\frac{D_T(0)}{D_T(B)} \approx C + (\omega\tau_2)^2$$

Assuming that tau is nearly constant in the relevant velocity range, we have

$$\tau_2^2 = \frac{\langle \tau v^2 \rangle \left\langle \frac{v^2}{\tau} \right\rangle}{\left\langle \frac{v^2}{\tau} \right\rangle^2} \approx \bar{\tau}^2$$

The transverse diffusion is thus expected to attain its minimum at the maximum tau, or at around the Ramsauer dip. Notice also that the drift velocity attains its maximum near there as expected.



The DL being different from the DT is unexpected and needs explanation.

Diffusion Revisited

Electric Anisotropy

The fact that the diffusion in the E-field direction differs from those in the other directions was first noticed by Wagner, Davis, and Hurst (1967). This is called the electric anisotropy. Since our previous result indicated that the DL is equal to the DT at $B=0$, some approximation we made to some E-dependent terms must have been inadequate to explain this phenomenon. We then need to go back to the scalar equation

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

with

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

and

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

By multiplying both sides by the kinetic energy of the electron and integrating

over the electron speed, we can translate the scalar equation into the following form

$$\frac{\partial}{\partial t} (n \langle \epsilon \rangle_v) + \frac{\partial}{\partial x} (n \langle \epsilon \mathbf{W} \rangle_v) = n \langle \mathbf{W} \rangle_v \cdot e\mathbf{E} - \int dv m v \sigma_{\text{coll}}$$

where

$$\epsilon := \frac{1}{2} m v^2$$

The equation expresses the conservation of energy. Recall that if collisions are all elastic and the speed of molecules can be neglected, we have

$$\sigma_{\text{coll}} \approx \sum_k 4\pi v^2 \frac{m}{M_k} v (n f_0) \nu_{m,k}$$

where

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

When a molecule is at rest, energy loss per collision is given by

$$\Delta\epsilon = \lambda_k \epsilon = 2 \frac{M_k m}{(M_k + m)^2} \epsilon \simeq 2 \frac{m}{M_k} \epsilon$$

where lambda is called the fractional energy loss.

Diffusion Revisited

Electric Anisotropy

The collision term then becomes

$$\int dv m v \sigma_{\text{coll}} \approx n \int dv (4\pi v^2) f_0 \overline{(\lambda\nu)} \epsilon = n \langle \epsilon \overline{(\lambda\nu)} \rangle_v$$

with

$$\overline{(\lambda\nu)} := \sum_k \lambda_k \nu_{m,k}$$

Putting these together, we get

$$\frac{\partial}{\partial t} (n \langle \epsilon \rangle_v) + \frac{\partial}{\partial x} (n \langle \epsilon \mathbf{W} \rangle_v) = n \langle \mathbf{W} \rangle_v \cdot e\mathbf{E} - n \langle \epsilon \overline{(\lambda\nu)} \rangle_v$$

Since we are dealing with a single electron in a quasi steady state, the L.H.S. may be ignored in considering a change in the scale of one mean free time. The eq. then reads

$$n \langle \mathbf{W} \rangle_v \cdot e\mathbf{E} = n \langle \epsilon \overline{(\lambda\nu)} \rangle_v$$

indicating local balance between the energy gain from the E-field and the loss due to collisions. Since the current density

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

includes the contribution from diffusion, so does the L.H.S. of the above equation.

Setting our coordinate axes in such a way that the E-field points to the 3rd axis direction and recalling that

$$\langle \mathbf{W}_E \rangle_v \cdot e\mathbf{E} = e\mu E^2$$

$$\langle \mathbf{W}_G \rangle_v \cdot e\mathbf{E} = -eE D \frac{1}{n} \left(\frac{\partial n}{\partial x_3} \right)$$

we can rewrite the energy balance eq. as

$$e\mu E^2 - eE D \frac{1}{n} \left(\frac{\partial n}{\partial x_3} \right) \approx \langle \epsilon \rangle_v \overline{(\lambda\nu)} (\langle \epsilon \rangle_v)$$

Denoting $\bar{\epsilon} = \langle \epsilon \rangle_v$ and expanding this eq. around the energy corresponding to the average energy at the peak of the electron spatial probability distribution where the derivative is zero, we have

$$e \frac{e}{m} \frac{1}{\nu_0 + \left(\frac{\partial \nu}{\partial \bar{\epsilon}} \right)_0 \Delta \bar{\epsilon}} E^2 - eE \frac{2\bar{\epsilon}_0}{3m} \frac{1}{\nu_0} \frac{1}{n} \left(\frac{\partial n}{\partial x_3} \right) \\ \approx (\bar{\epsilon}_0 + \Delta \bar{\epsilon}) \left[\overline{(\lambda\nu)}_0 + \left(\frac{\partial \overline{(\lambda\nu)}}{\partial \bar{\epsilon}} \right)_0 \Delta \bar{\epsilon} \right]$$

where use has been made of

Diffusion Revisited

Electric Anisotropy

$$\mu = \frac{e}{m} \langle \tau \rangle \approx \frac{e}{m\nu} \quad \text{and} \quad D = \frac{1}{3} \langle v^2 \tau \rangle \approx \frac{2\bar{\epsilon}_0}{3m\nu_0}$$

The energy balance eq. can be solved for the energy shift as

$$\Delta\bar{\epsilon} = -\frac{2\bar{\epsilon}_0^2}{3eE \left[1 + \left(\frac{\bar{\epsilon}_0}{\nu_0} \right) \left(\frac{\partial\nu}{\partial\bar{\epsilon}} \right)_0 + \left(\frac{\bar{\epsilon}_0}{(\lambda\nu)_0} \right) \left(\frac{\partial(\lambda\nu)}{\partial\bar{\epsilon}} \right)_0 \right]} \frac{1}{n} \left(\frac{\partial n}{\partial x_3} \right)$$

At the leading edge, where the density has a -ve slope, the energy shift is +ve, and at the trailing edge, the energy shift is -ve.

The energy is hence higher at the leading edge and lower at the trailing edge than at the center. This energy shift induces the variation of mobility along the E-field:

$$\mu = \frac{e}{m\nu} \approx \frac{e}{m\nu_0} \left[1 - \frac{1}{\nu_0} \left(\frac{\partial\nu}{\partial\bar{\epsilon}} \right)_0 \Delta\bar{\epsilon} \right]$$

Denoting

$$\gamma = \frac{\bar{\epsilon}_0}{\nu_0} \left(\frac{\partial\nu}{\partial\bar{\epsilon}} \right)_0 \quad \text{and} \quad \gamma' = \frac{\bar{\epsilon}_0}{(\lambda\nu)_0} \left(\frac{\partial(\lambda\nu)}{\partial\bar{\epsilon}} \right)_0$$

we have

$$\mu \approx \frac{e}{m\nu_0} \left[1 + \frac{2\gamma\bar{\epsilon}_0}{3eE(1+\gamma+\gamma')} \frac{1}{n} \left(\frac{\partial n}{\partial x_3} \right) \right]$$

Depending on the sign of "gamma", the variation induces a bunching (+ve) or debunching (-ve) effect and hence makes the longitudinal diffusion different from the transverse one.

Putting these into

$$n \langle W \rangle_v = n \mu E - D \frac{\partial}{\partial x} n$$

and taking the 3rd component, we have

$$\begin{aligned} n \langle W_3 \rangle_v &= n \mu E - D \frac{\partial}{\partial x_3} n \\ &= n \frac{e}{m\nu_0} E - D \left[1 - \frac{\gamma}{1+\gamma+\gamma'} \right] \frac{\partial}{\partial x_3} n \end{aligned}$$

which implies

$$D_L = D \left[1 - \frac{\gamma}{1+\gamma+\gamma'} \right]$$

The formula shows that $D_L = D_T(B=0)$ where "gamma"=0, the collision freq. attains its minimum (=tau maximum) meaning near the Ramsauer dip as we have seen for P5.