How do electrons move in a gas?

We would like to know:

- How fast are the electrons ?
- Will they move in a straight line ?
- Are they absorbed ?
- Do they produce showers ?

For this, we will have to understand first:

- Distances between gas molecules
- Mean free path of electrons
- Interactions between electrons and gas

Amedeo Avogadro (1776-1856)

Distances in gases

Number of Ar atoms in a cm³:
 Avogadro's number: 6.0
 Atomic weight of Ar: 40
 Density of Ar: 1.0

~Loschmidt's number:

6.022 10^{23} atoms/mole ÷ 40 g/mole × 1.662 10^{-3} g/cm³ = 2.5 10^{19} atoms/cm³



amedeo avogadro

Distance between neighbouring Ar atoms:

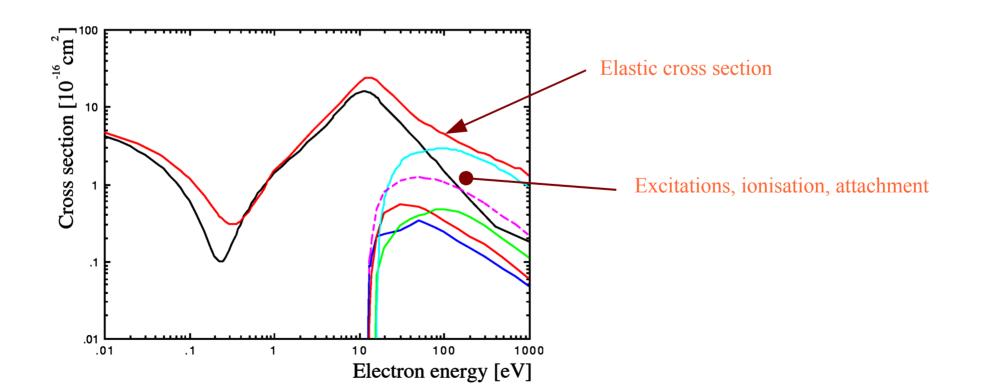
► How about \overline{e} . $\frac{19}{2}$ = $\frac{19}{2}$ = $\frac{19}{2}$ = $\frac{19}{2}$ = $\frac{19}{2}$ = $\frac{19}{2}$ = $\frac{1}{2}$ = \frac

Josef Loschmidt(1821-1895)



Cross section of argon

Cross section in a hard-sphere model:
 Radius: ~70 pm (http://www.webelements.com)
 Surface:
 Simplified cross sections used by Magboltz.⁻¹⁶ cm²



Mean free path in argon

We know already that: Cross section of 1 atom: $\sigma \approx 1.5 \ 10^{-16} \ \mathrm{cm}^2$ Atoms per volume:

 $\mathscr{L} \approx 2.5 \ 10^{19} \, \mathrm{atoms/cm^3}$

- Mean free path for an electron ?
 - An electron hits all atoms of which the centre is less than a cross section radius from its path
 - \triangleright Over a distance L, the electron hits $\mathcal{L}\sigma L$ atoms
 - ► Hence, the mean free path is $\lambda_{\rho} = 1/(\mathscr{L}\sigma) \approx 2.7 \ \mu m$
 - Much larger than the distance between atoms, 3.5 nm and typical gas molecule diameters, 140-600 pm.

Drift velocity in electric fields

Imagine that an electron stops every time it collides with a gas molecule and then continues along *E*.
 To cover a distance , it will need a time *t*:

$$= \frac{1}{\text{Formexample}} t^2 = \lambda_{\text{e}}, \quad i.e. \quad t = \sqrt{\frac{2\lambda_{\text{e}}m_{\text{e}}}{qE}}, \quad i.e. \quad \overline{v} = \frac{\lambda_{\text{e}}}{t} = \sqrt{\frac{\lambda_{\text{e}}qE}{2m_{\text{e}}}}$$

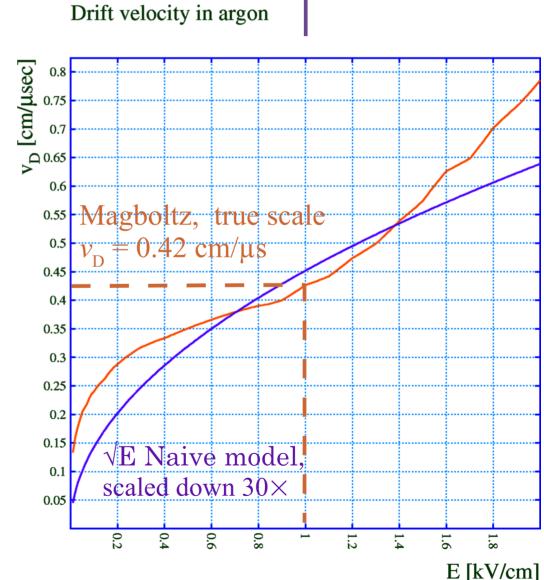
$$\overline{v} = \sqrt{\frac{1.910^{-6} \text{ m } 1.610^{-19} \text{ C } E[\text{V/m}]}{2 \ 9.110^{-31} \text{ kg}}}$$
$$\approx 13 \text{ cm/}\mu \text{ s } \text{ for } E = 1 \text{ kV/cm}$$

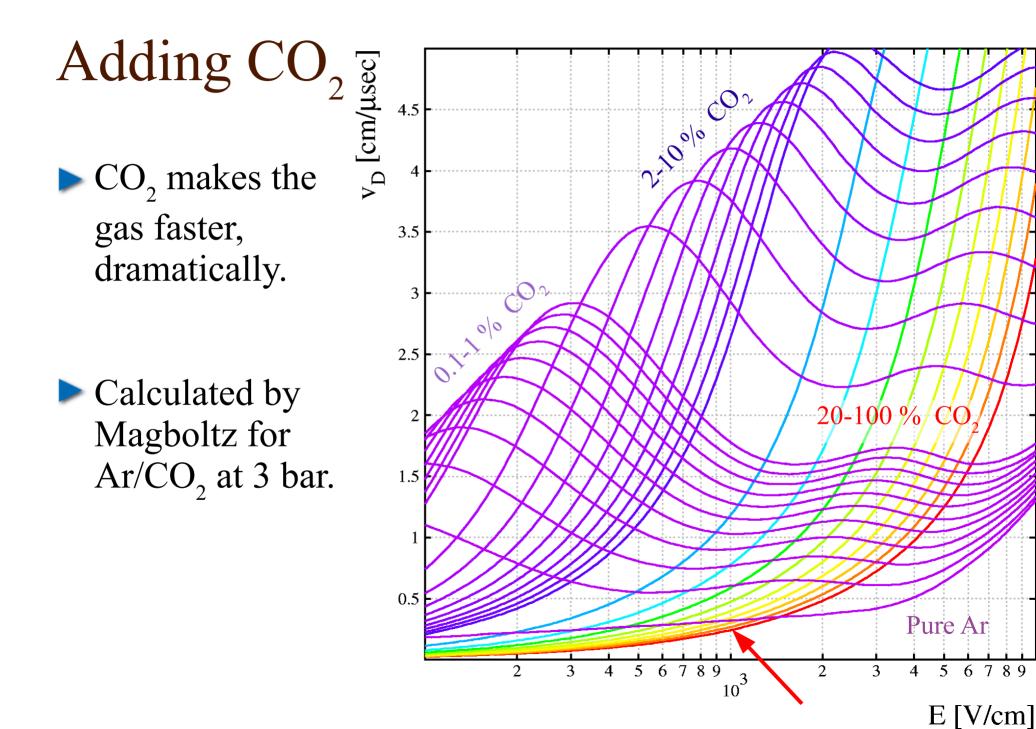
Drift velocity in argon

- Compare with a Magboltz calculation for pure argon:
 - \triangleright *E* dependence is OK;

BUT

the velocity is vastly overestimated !



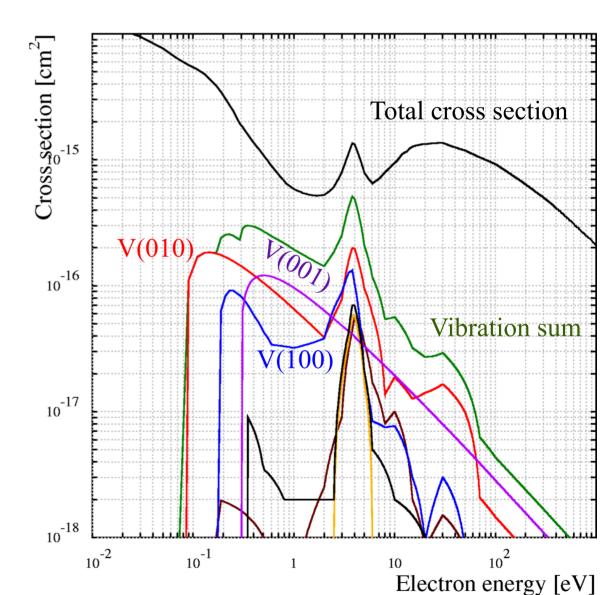


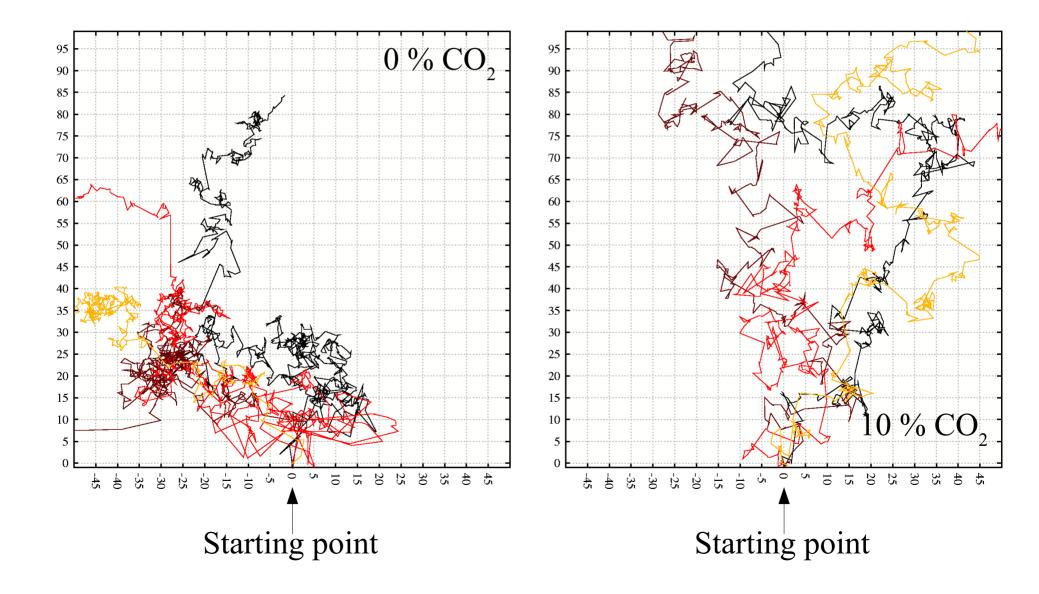
 CO_2 – vibration modes

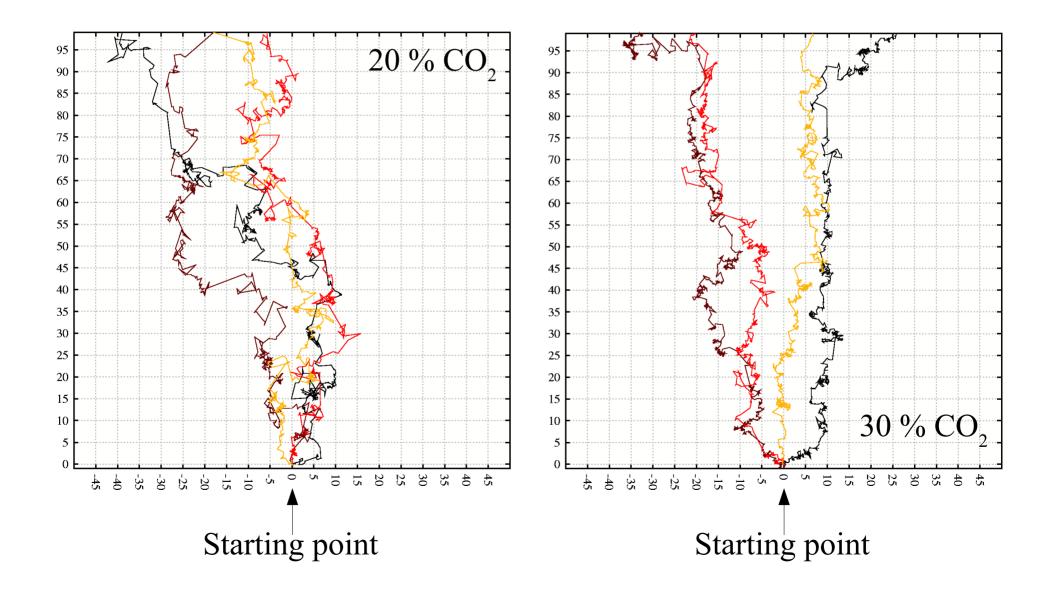
► CO_2 is linear: ► O - C - O

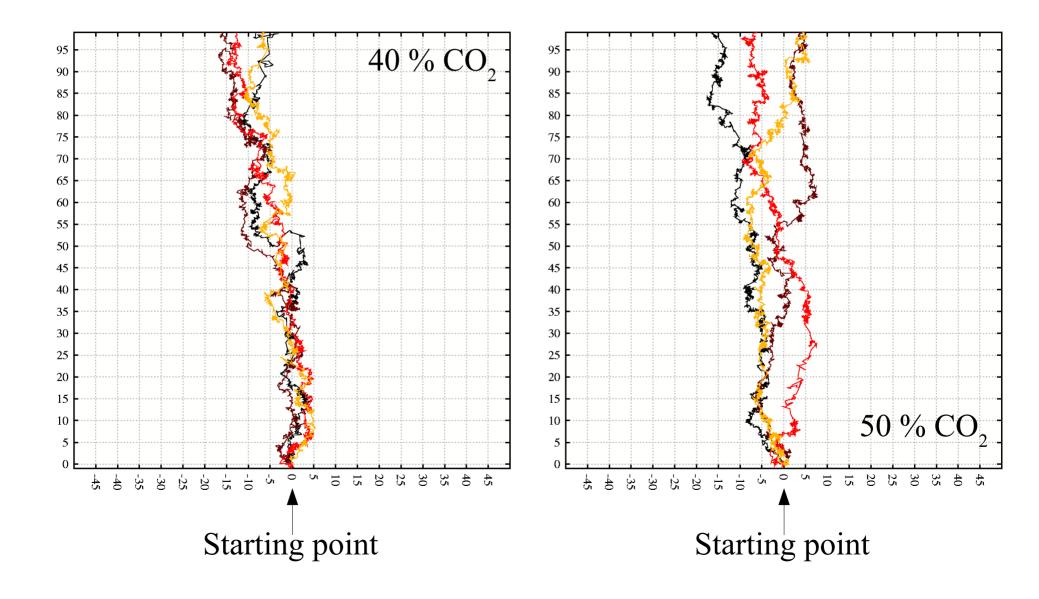
Vibration modes are numbered V(*ijk*) *i*: symmetric, *j*: bending, *k*: anti-symmetric.

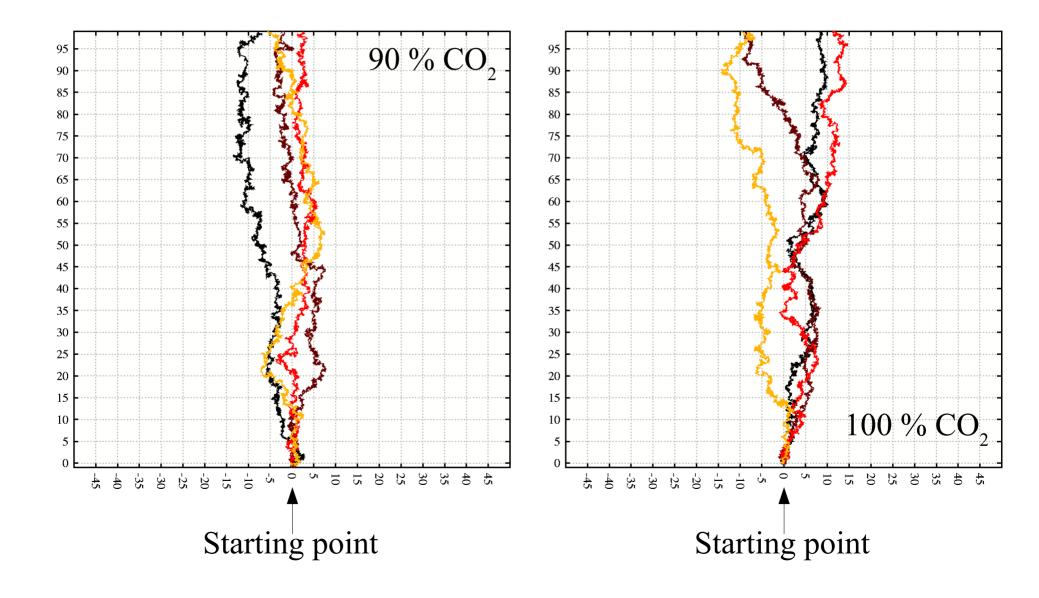
Vibrations V(ijk)





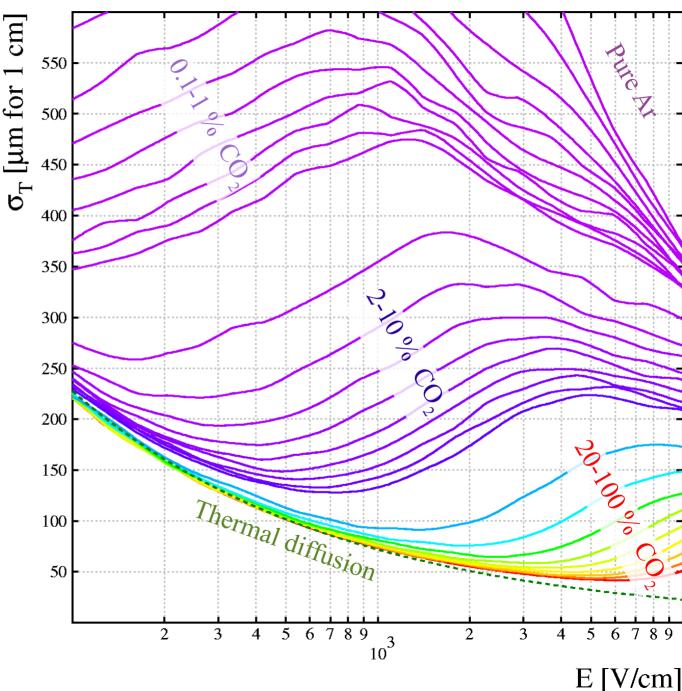






much reduced by CO₂.

Calculated by Magboltz for Ar/CO_{2} at 3 bar.



Magboltz

- ► A large number of cross sections for 60 molecules...
 - All noble gases, *e.g.* argon:
 - elastic scattering,
 - 44 excited states and
 - ionisation.
 - > Numerous organic gases, additives, $e.g. CO_2$:
 - elastic scattering,
 - 44 inelastic cross sections (vibrations, rotations, polyads)
 - 35 super-elastic cross sections,
 - 6 excited states,
 - attachment and
 - ionisation.

LXcat

• LXcat (pronounced *elecscat*) is an open-access website for collecting, displaying, and downloading ELECtron SCATtering cross sections and swarm parameters (mobility, diffusion coefficient, reaction rates, etc.) required for modeling low temperature plasmas. [...]"

URL: http://www.lxcat.laplace.univ-tlse.fr/

Arthur V. Phelps

1962: Numerical e⁻ transport



Iterative approach, allowing for inelastic cross section terms:
 educated guess of cross sections (elastic & inelastic);
 numerically solve the Boltzmann equation (no moments);
 compare calculated and measured mobility and diffusion;
 adjust cross sections.

"... more than 50,000 transistors plus extremely fast magnetic core storage. The new system can simultaneously read and write electronically at the rate of 3,000,000 bits of information a second, when eight data channels are in use. In 2.18 millionths of a second, it can locate and make ready for use any of 32,768 data or instruction numbers (each of 10 digits) in the magnetic core storage. The 7090 can perform any of the following operations in one second: 229,000 additions or subtractions, 39,500 multiplications, or 32,700 divisions. " (IBM 7090 documentation)

[L.S. Frost and A.V. Phelps, *Rotational Excitation and Momentum Transfer Cross Sections for Electrons in* H_2 *and* N_2 *from Transport Coefficients*, Phys. Rev. **127** (1962) 1621–1633.]



Transport equation

The momentum transfer cross section appears in the Boltzmann equation solved for transport parameters:

 $\frac{E^2}{3} \frac{d}{du} \left(\frac{u}{NQ_m} \frac{df}{du} \right) + \frac{2m}{M} \frac{d}{du} (u^2 NQ_m f) + \frac{2mkT}{M_c} \frac{d}{du} \left(u^2 NQ_m \frac{df}{du} \right) + \sum_j (u+u_j) f(u+u_j) NQ_j(u+u_j) - uf(u) N_j \sum_j Q_j(u) + \sum_j (u-u_j) f(u-u_j) NQ_{-j}(u-u_j) - uf(u) N \sum_j Q_{-j}(u) = 0.$ Convergies is traditionally derived from transport parameters (drift velocity and diffusion).

Literature: LS Frost and AV Phelps (1962) 10.1103/PhysRev.127.1621 and later publications by the same group.

LXcat people

Art Phelps,
Leanne Pitchford – Toulouse,
Klaus Bartschat – Iowa,
Oleg Zatsarinny – Iowa,
Michael Allan – Fribourg,
Steve Biagi

Leanne Pitchford

Michael Allan

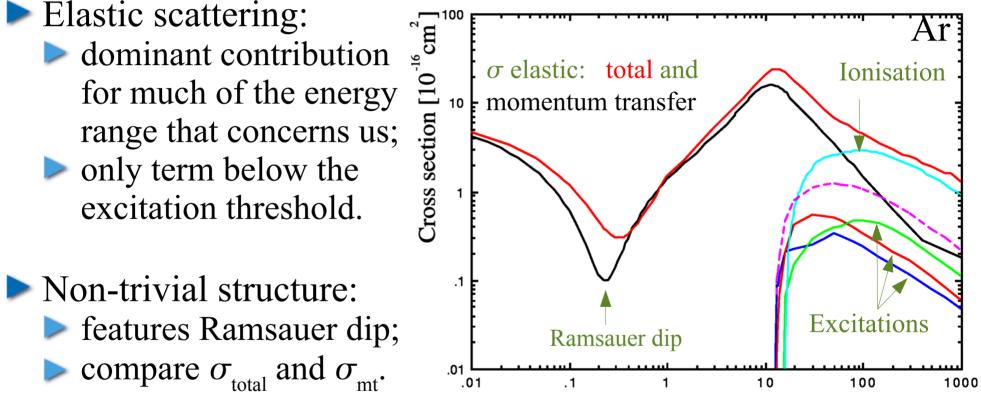




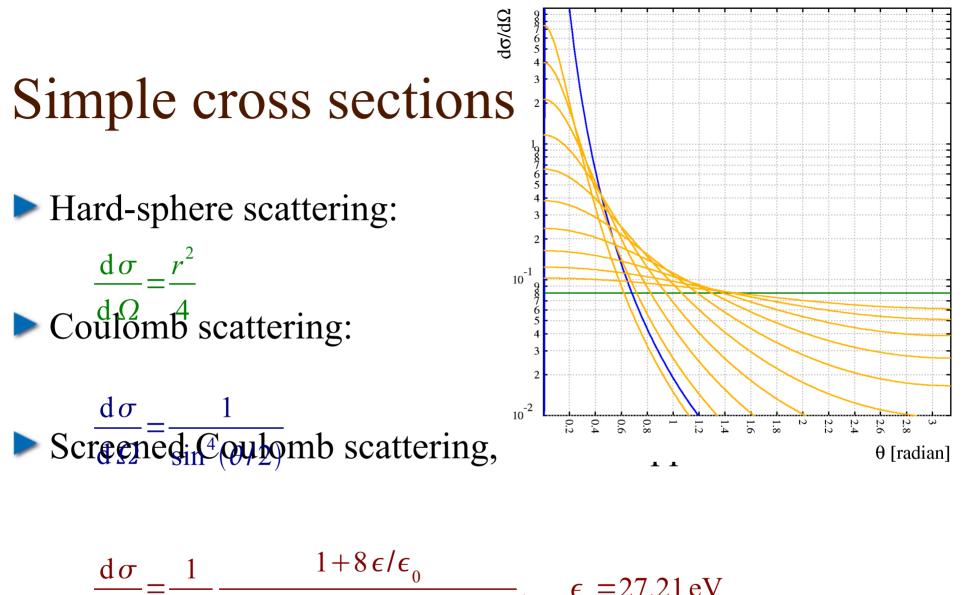




How isotropic is e⁻ scattering on Ar ?



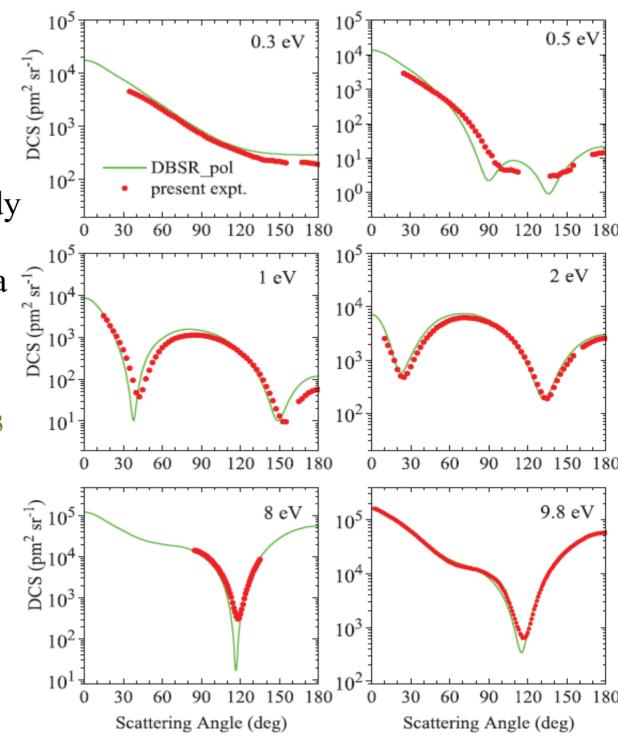
Electron energy [eV]



$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \frac{1}{4\pi} \frac{1 + 8\epsilon/\epsilon_0}{\left(1 + 4\epsilon/\epsilon_0 - 4\epsilon/\epsilon_0\cos\theta\right)^2}, \quad \epsilon_0 = 27.21\,\mathrm{e}$$

Krypton data

A remarkable joint study with high-precision experimental data and a theoretical model has just been published:
 O. Zatsarinny et al. (2011) 10.1103/PhysRevA.83.032713



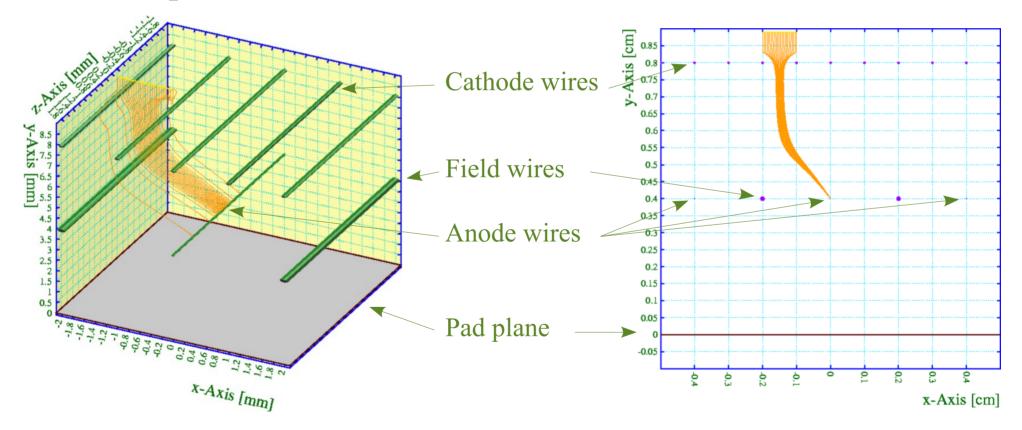
Scale \gg mean free path (> 1 mm)

- For practical purposes, electrons from a given starting point reach the same electrode – but with a spread in time and gain.
- Electrons transport is treated by:
 - integrating the equation of motion, using the Runge-Kutta-Fehlberg method, to obtain the path;
 - integrating the diffusion and Townsend coefficients to obtain spread and gain.

This approach is adequate for TPCs, drift tubes etc.

Runge-Kutta-Fehlberg integration

Example: a TPC read-out cell



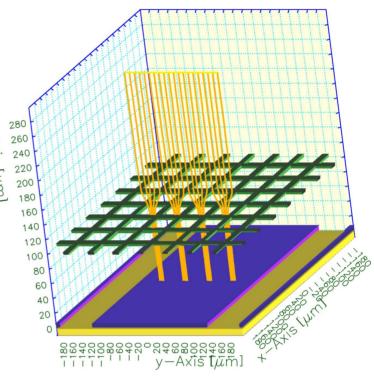
Scale > mean free path (100 μ m - 1 mm)

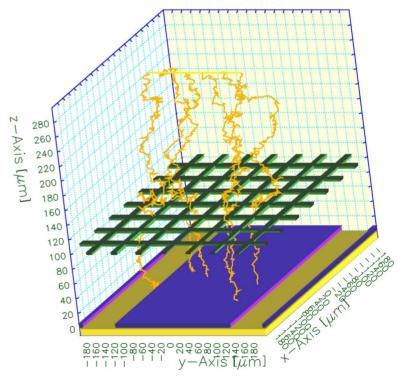
- Electrons from a single starting point may end up on any of several electrodes.
- Calculations use Monte Carlo techniques, based on the mean drift velocity and the diffusion tensor computed by microscopic integration of the equation of motion in a constant field. Gain depends on the path.
- This approach is adequate as long as the drift field is locally constant – a reasonably valid assumption in a Micromegas but less so in a GEM.

Analytic vs Monte Carlo

Analytic integration:
 Runge-Kutta-Fehlberg technique;
 automatically adjusted step size;
 optional integration of diffusion, multiplication and losses.

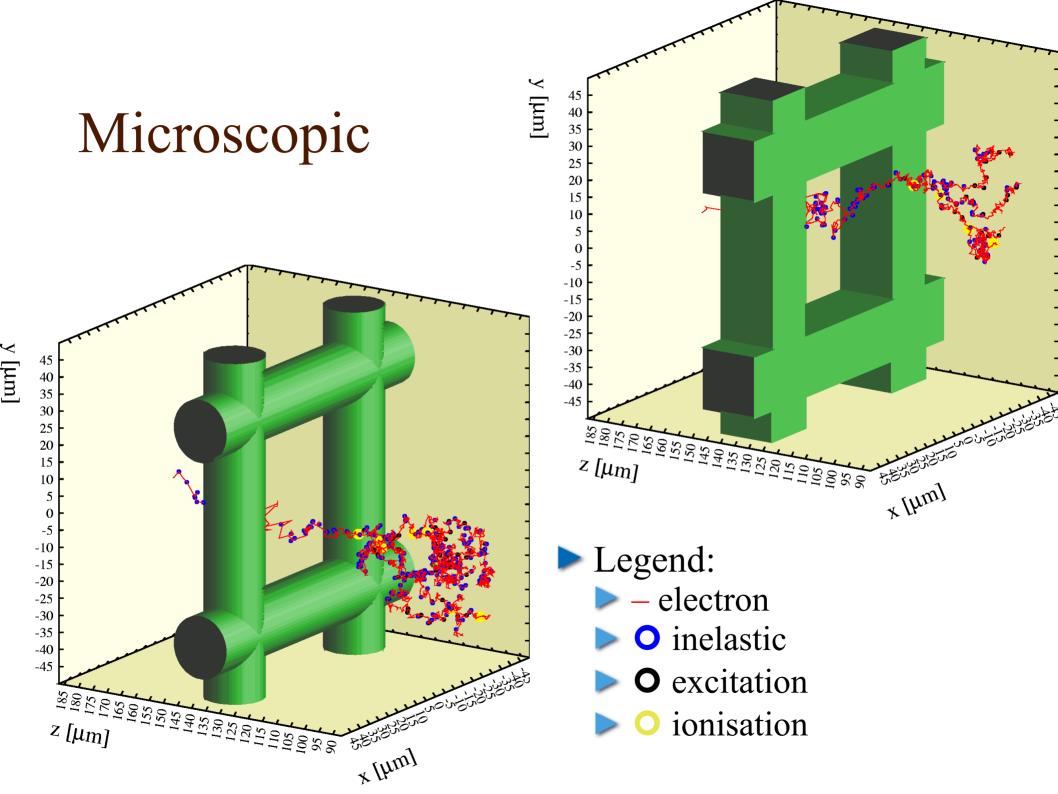
 Transport table-based Monte Carlo:
 non-Gaussian in accelerating, divergent and convergent fields;
 step size has to be set by user.
 Replaced by molecular simulation.





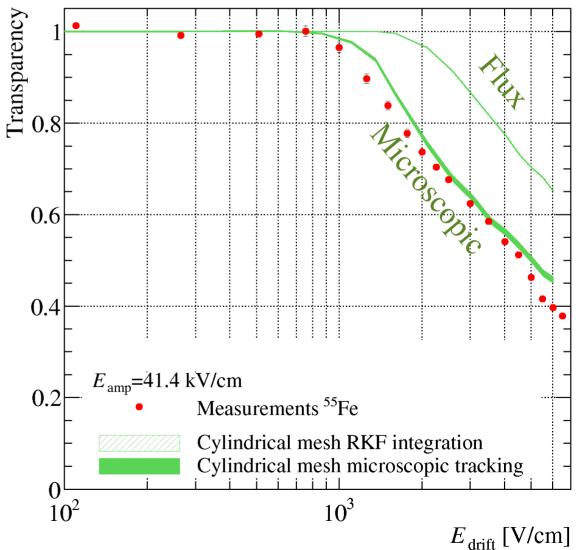
Scale ~ mean free path (1-100 μ m)

- At this scale, where the mean free path approaches the characteristic dimensions of detector elements, free flight between collisions is no longer parabolic.
- The only viable approach seems to be a molecular simulation of the transport processes.
- Can be achieved by running Magboltz in the detector field, rather than in a constant field as is done when preparing classic transport tables.



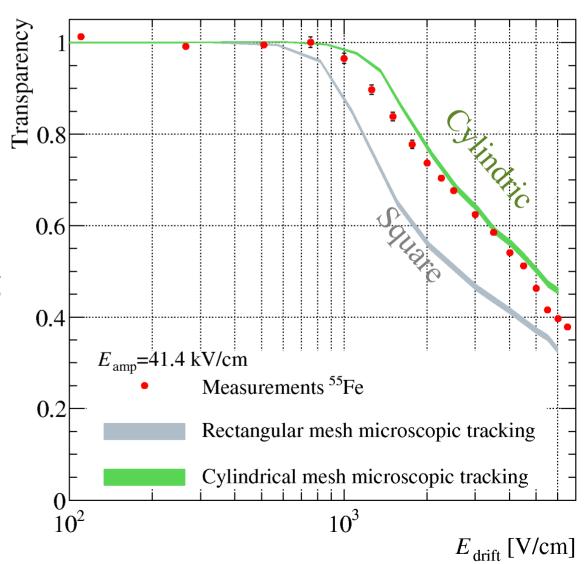
Flux vs microscopic?

- A diffusion-free flux argument does not reproduce the data.
- The microscopic approach works.
- Calculations done using finite elements.



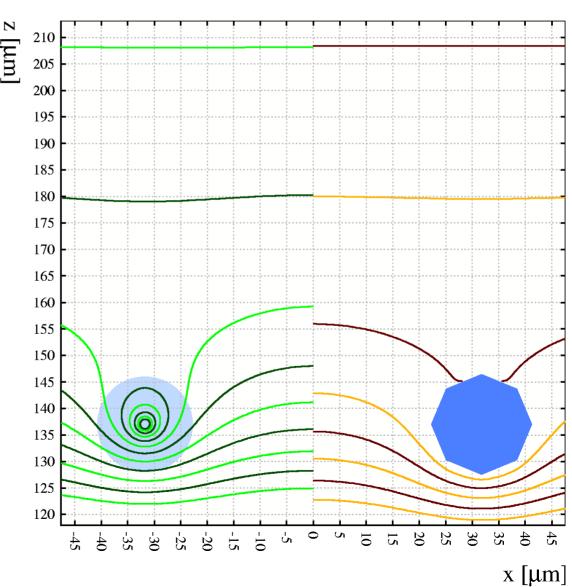
Square mesh wires ?

- Square wires are much simpler to model than cylindric wires – but this is an inadequate simplification.
- Calculations done using finite elements.



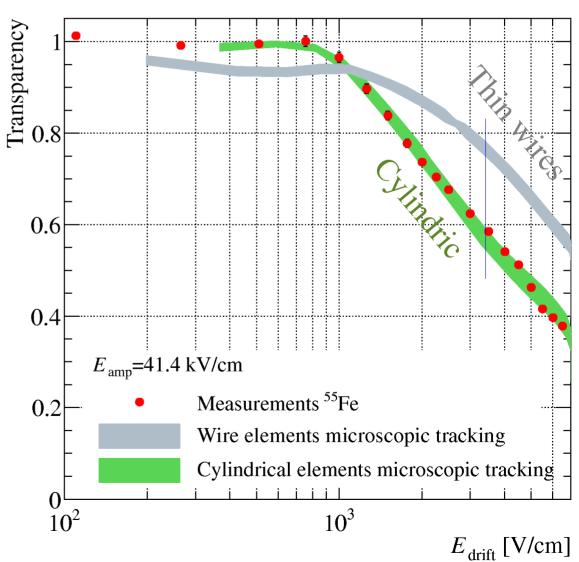
Dipole moment of the mesh

Compare equipotentials $\underline{E}_{drift} = 3.3 \text{ kV/cm}$: thin-wire elements overestimate the transparency by 15 %.



Thin-wire approximation ?

- The thin-wire approximation is usual in wire chambers – but is not adequate here.
- Calculations done using neBEM.



Attachment

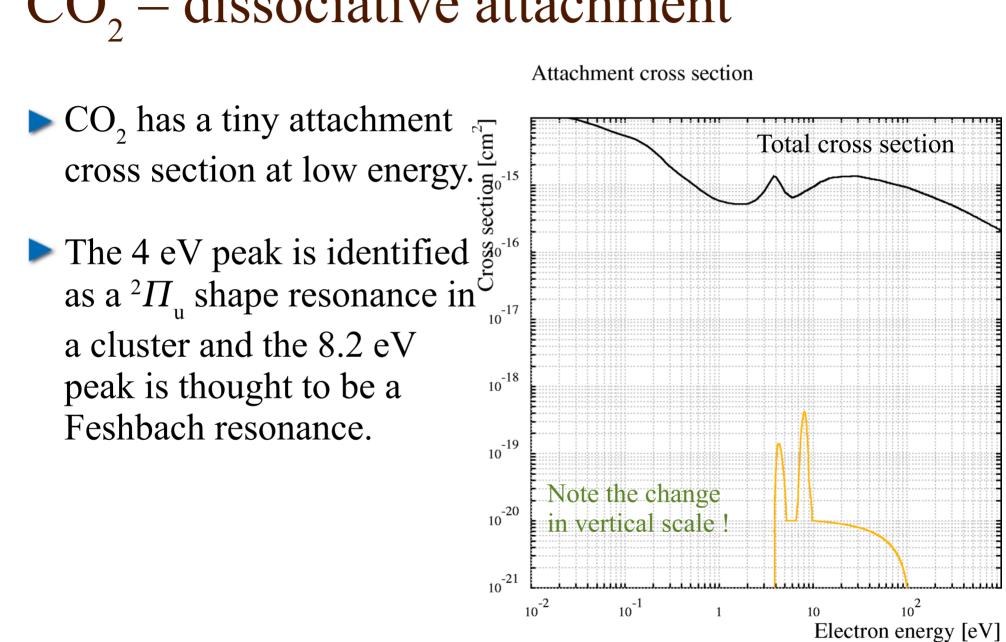
- Some of the quencher gases have the potential of attaching electrons.
- Examples include:
 - ► O_2 : mostly 3-body O_2^- and at higher ϵ 2-body dissociative;
 - > H₂O: [H₂O]_n has positive electron affinity, H₂O does not;
 - > CF_4 : mostly dissociative $F^- + CF_3$, $F + CF_3^-$ (below 10 eV);
 - > SF₆: SF₆⁻ up to 0.1 eV, $\sigma = 10^{-18}$ cm², then F⁻ + SF_n⁻ (n=3, 4, 5)
 - \triangleright CS₂: negative ion TPC;
 - \triangleright CO₂: O⁻, [CO₂]⁻_n but no CO₂⁻ (4 eV and 8.2 eV).

Attachment in CO₂

- ► Linear CO₂ with an extra e⁻ is instable ($\tau \ll 1$ ps) and has negative affinity ($\epsilon_{VEA} \approx -3.8 \text{ eV}$): low energy e⁻ collisions cause dissociative attachment, producing O⁻ but not CO₂⁻.
- ► With an e⁻ added, a bent structure (134°) is favoured. This has a long lifetime ($\tau \approx 90 \ \mu s$) but still has a *negative* electron affinity ($\epsilon_{AEA} \approx -0.6 \ eV$) and is metastable.
- Attachment of electrons works in $[CO_2]_n$ clusters where vibration and rotation modes can absorb excess energy.

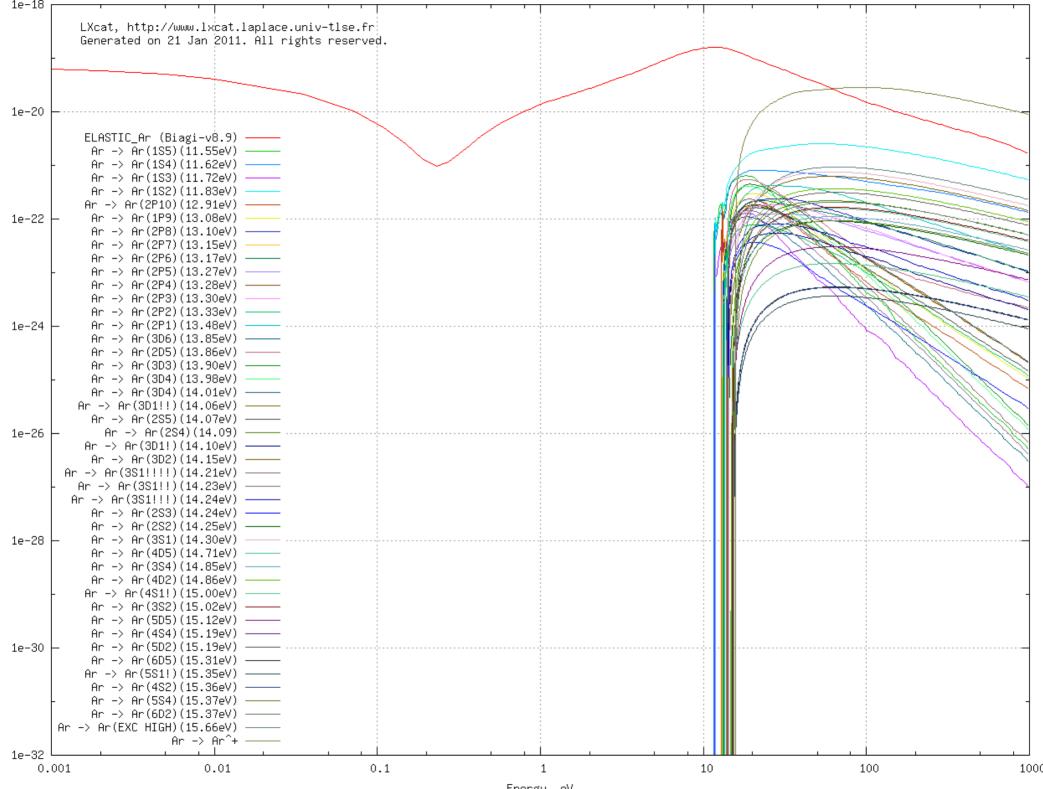
CO_{2} – dissociative attachment

Attachment cross section



Phase 3: Gain

- After transport, we still have most probably 40 electrons per cm of gas. We need to detect them. If we collect them on an electrode over 1 µsec, the current will be:
- I=40 × 1.610⁻¹⁹ C / 10⁻⁶ s=6.4 pA.
 Maybe manageable nowadays, but certainly not comfortable. Amplification is required.
- Amplification calls for fields where the energy after a mean free path > ionisation energy of 15.7 eV (in Ar).



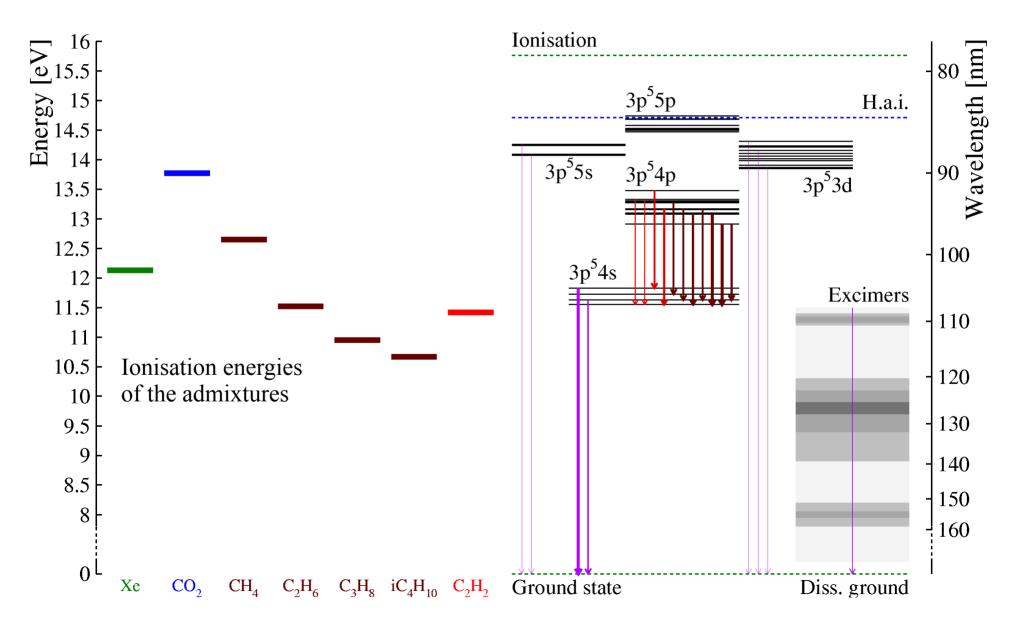
R

section

Cross

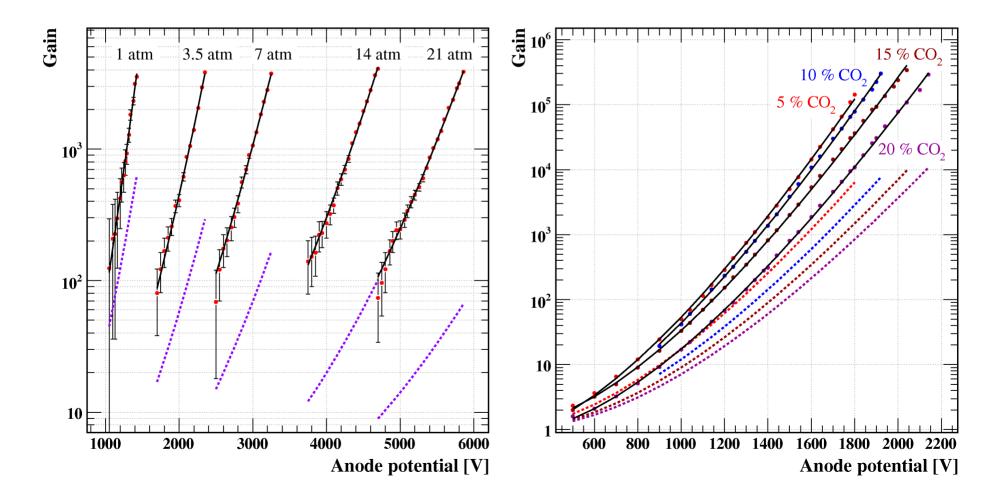
Energy, eV

Level diagram argon and admixtures



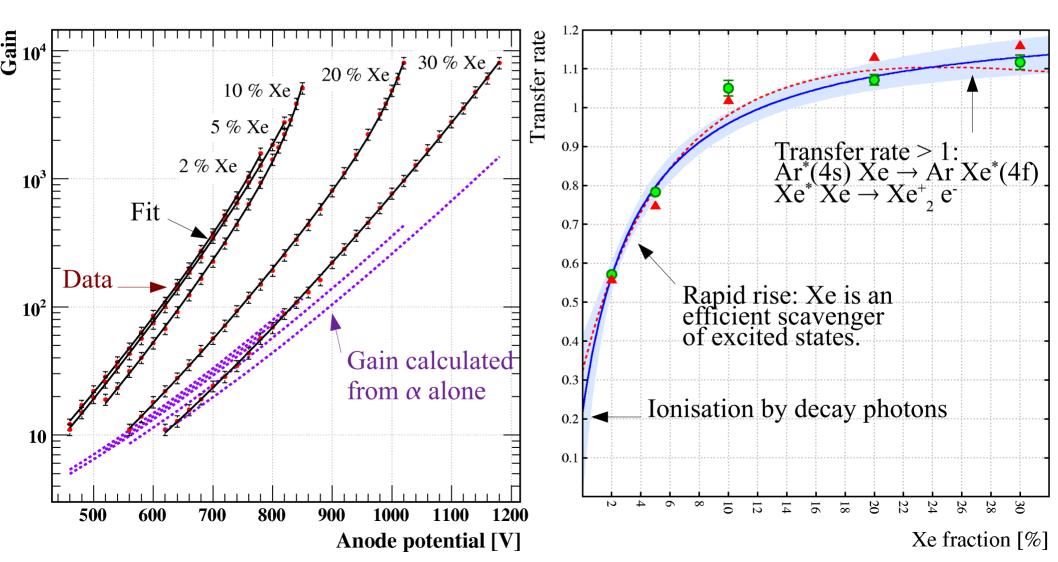
Importance of Penning transfer

► Ar^{*} 4p, 3d ... \rightarrow CH₄⁺ + e⁻ ► Ar^{*} 3d ... \rightarrow CO₂⁺ + e⁻



Penning transfer in Ar-Xe

Ar 4*p*, 3*d* and higher above the Xe ionisation threshold.



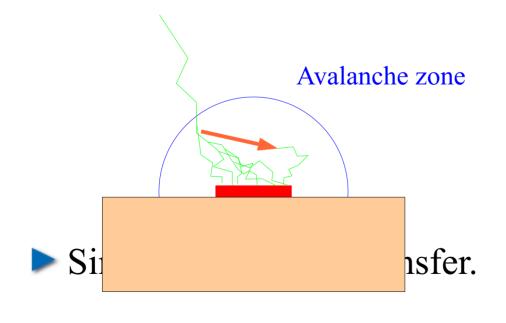
Photon feedback

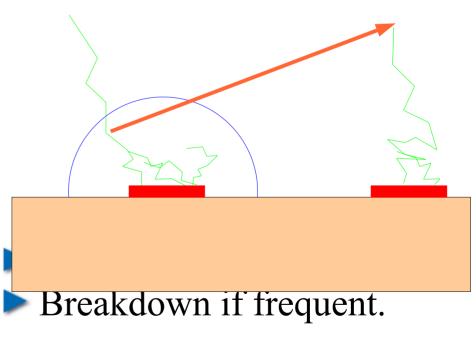
- Some excited states return to ground by emitting VUV photons which may be capable of ionising the quencher.
- Such photons have a high probability of repeatedly being absorbed and re-emitted by the noble gas: radiation trapping.
- Eventually, after many absorption/emission cycles, the photons are absorbed by a quencher gas molecule.

Photon feedback

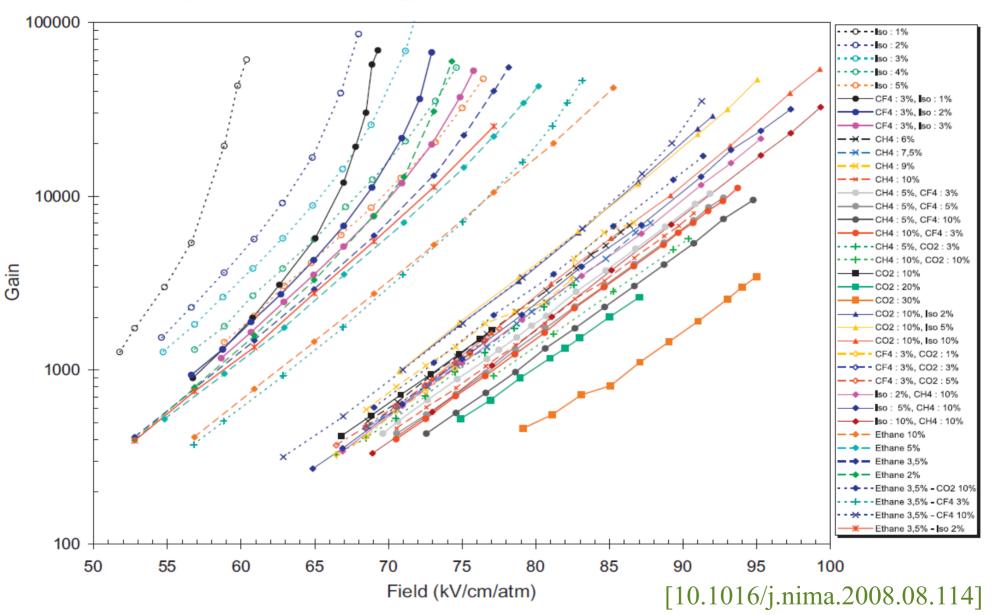
A γ absorbed inside the avalanche enhances the gain:

A y leaving the avalanche zone can start a complete new avalanche:





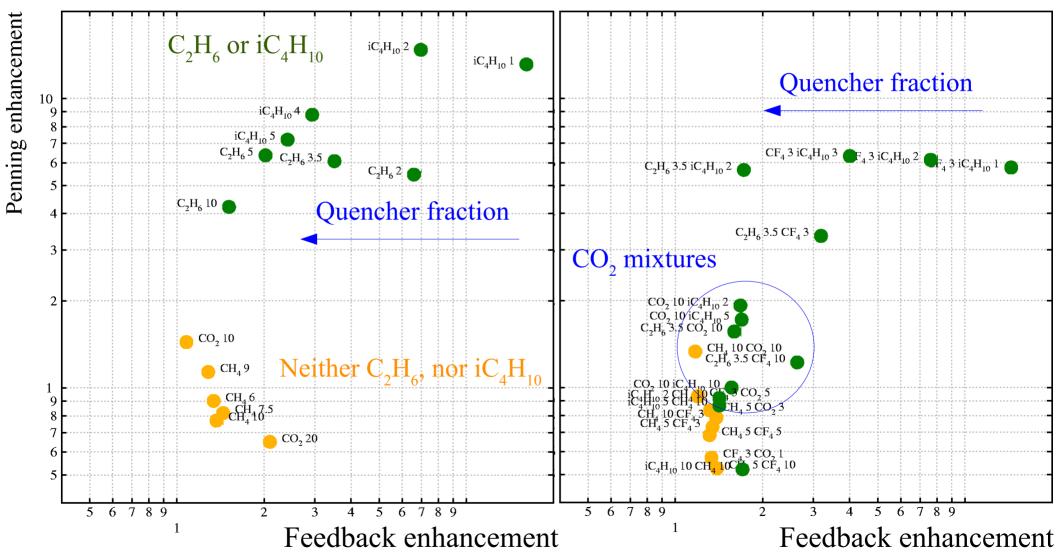
Saclay Ar compilation



Penning vs feedback enhancement

Binary mixtures

Ternary mixtures



Which quenchers are affected ?

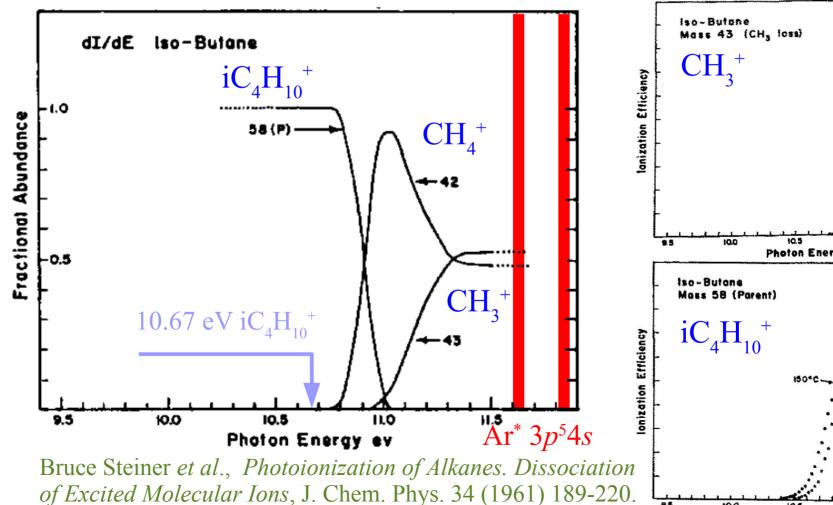
Energy

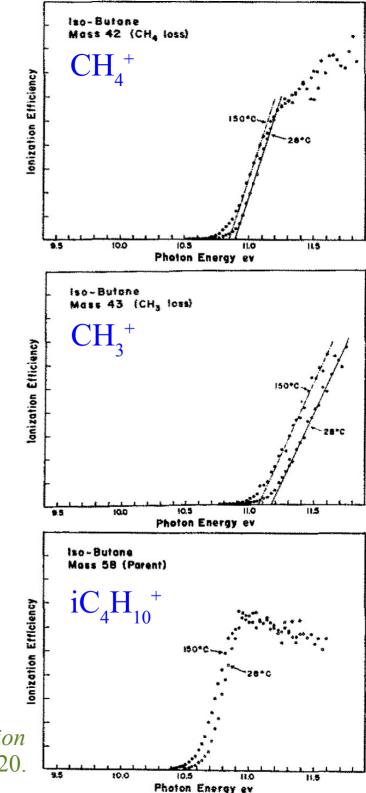
The admixture molecules need to have an ionisation energy below the Ar excitation levels:

10.67 eV C,H₆: 11.52 eV $Ar^* 3p^5 4s:$ $11.55_{\rm m}$, $11.62_{\rm r}$, $11.72_{\rm m}$, $11.83_{\rm r}$ eV dominant 12.99 eV CH_{A} : Ar* $3p^{5}4p$: ~13 eV; non-radiative 13.77 eV CO₂: Ar* $3p^53d$: ~14 eV; CF_{A} : 15.90 eV

iC₄H₁₀ photo-ionisation

▶ Dominated by CH_3^+ and CH_4^+ loss.





Origin of the gain

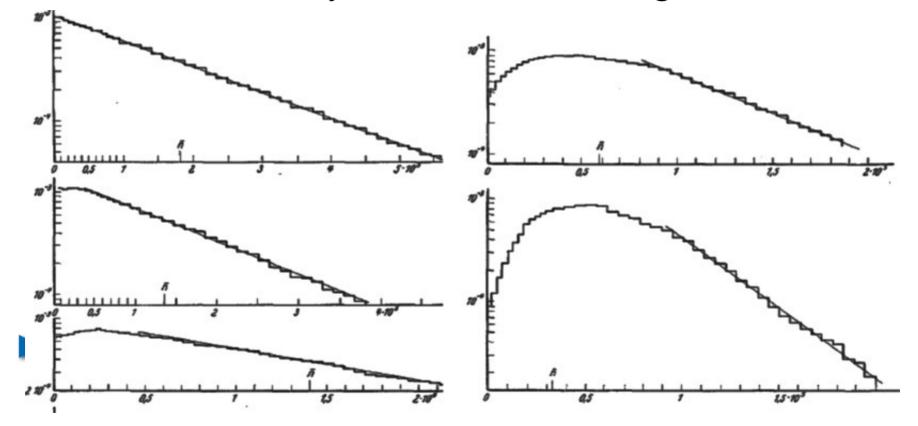
- ▶ Photo-ionisation of the admixture by $Ar^* 3p^54s$ photons occurs with iC_4H_{10} , is marginal with C_2H_6 and should not occur with e.g. CO_2 and CH_4 .
- The C_2H_6 and iC_4H_{10} mixtures owe their high gain to the Penning effect and, at small C_2H_6 and iC_4H_{10} percentages, to gas feedback.
- Feedback is suppressed and the Penning effect is reduced in the presence of CO₂.

Avalanche statistics

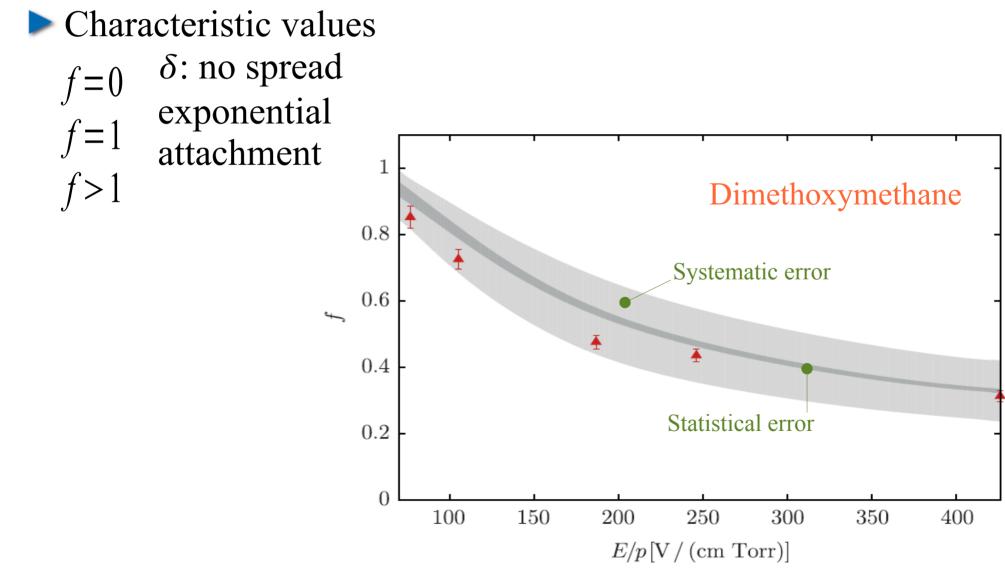
- The simplest avalanche growth models lead to exponential avalanche size distributions.
- This neglects the effects of
 - minimum path length before a new ionisation;
 - energy loss in inelastic collisions;
 - excitations;
 - Penning effect;
 - attachment.
- This results in desirable modifications of the avalanche size distribution.
- DOI: 10.1016/j.nima.2010.09.072

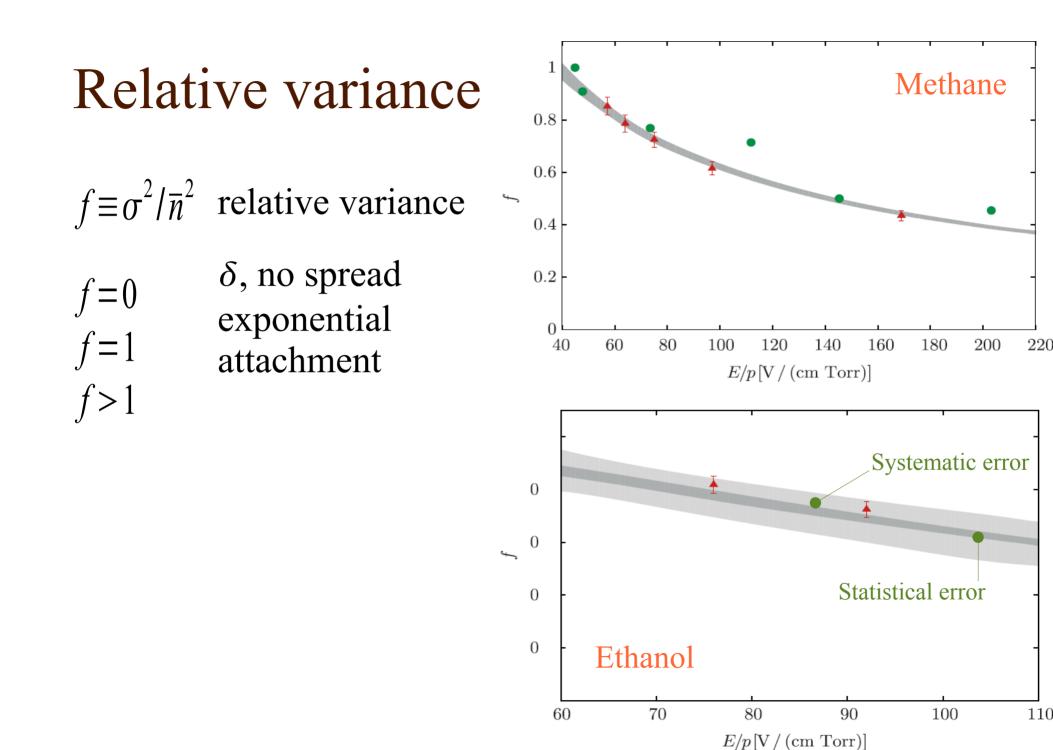
Avalanche size distributions

► Data for dimethoxymethane at increasing E field:



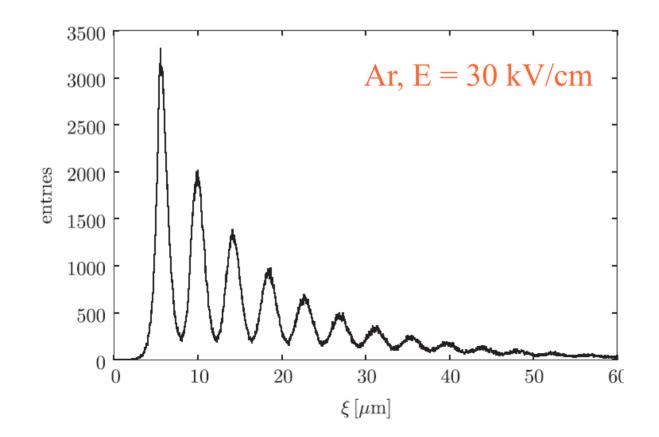
Relative variance $f \equiv \frac{\sigma^2}{\overline{n}^2}$





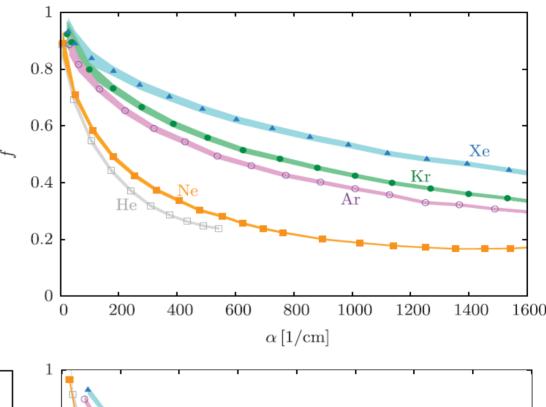
Ionising collision spacing

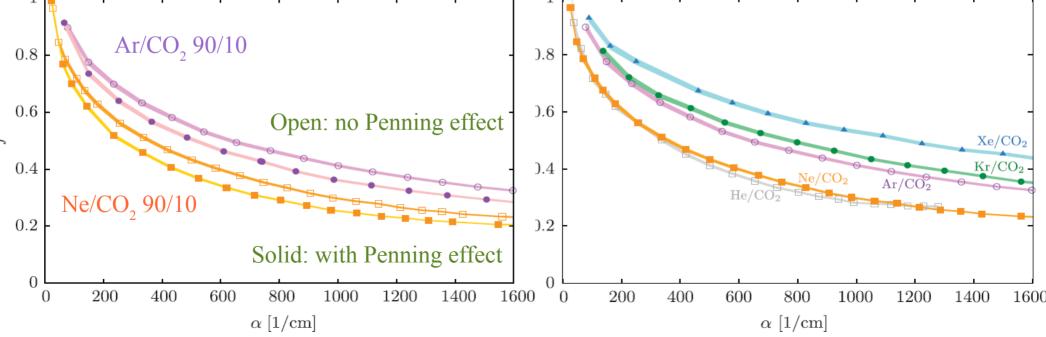
The inelastic region and the "fence" of excitations protecting the ionisation force an electron to make sometimes numerous attempts to ionise:



Trends

Quenchers: more inelastic & `less ionisation → larger f;
 Penning transforms excitation into ionisation → smaller f.





Phase 4: Signals

Remains reading the signals induced by the electrons and ions moving around in the chamber.

Signals

Properties of the current induced in an electrode:
 proportional to the charge Q;
 proportional to the valuatity of the abargant.

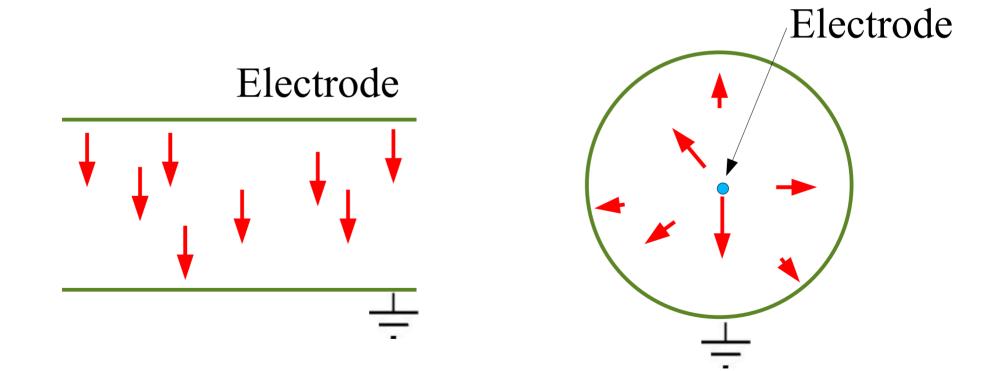
- > proportional to the velocity of the charge \vec{v} ;
- dependent on the electrode and the geometry.
- This leads to the following ansatz:

 $I = -Q\vec{v_{d}} \cdot \vec{E}_{w}$

- The geometry is contained in \vec{E} , necessarily a vectorial quantity, the *weighting field*. Each electrode has its own weighting field.
- The sign is mere convention.

Weighting field – examples

The weighting field is often easy to guess:



Weighting fields – more in general

Claim: \vec{E}_{w} can be computed from the potential:

read-out electrode set to 1;

all other electrodes set to 0;

 \triangleright note ... 0 and 1, not 0 V and 1 V !

This is plausible considering examples, and is proven using Green's reciprocity.

George Green's father's mill (Nottingham)

1828: George Green's work



 The basic techniques to solve electrostatics problems, still used today, were published by George Green in:
 "An Essay on the Application of Mathematical Analysis to the Theories of Electricity and Magnetism".

"(...) it was written by a young man, who has been obliged to obtain the little knowledge he possesses, at such intervals and by such means, as other indispensable avocations which offer but few opportunities of mental improvement, afforded."

only 55 copies were printed, only for the subscriber'S.

[Original printed for the author by T Wheelhouse, Nottingham (1828). Facsimile Mayer & Müller, Berlin (1889), scanned by Google books.]

Green's function technique

The embryo of the Green's function technique is found in article 7 (p 21):

Substituting for P', the value which results from this equation, in that immediately preceding we obtain

$$V' = -\int \frac{dxdydz \delta V}{4\pi r'} + \int \frac{\rho d\sigma}{r},$$

which, by means of the equation (3) art. 3, becomes

In this expression, one recognises the Green's function $a_{\text{S}}^{\text{the orizontal lines over the quantities, indicating that they belong to the surface itself.}$

$$V = \int_{S} \rho \frac{1}{r} dx + \oint_{\partial S} (V \nabla \frac{1}{r} - \frac{1}{r} \nabla V) \cdot dn$$

George Green (1793-1841)

Green's identities



► Green starts from what is now known as his 2nd identity:

Let U and V be two continuous functions of the rectangular co-ordinates x, y, z, whose differential co-efficients do not become infinite at any point within a solid body of any form whatever; then will

In current notation, using the divergence theorem, dw points

Михайло Васильович Остроградський in 1826, stated by Gauss in 1813, known to Lagrange in 1762:

Serves $a_{s}^{(U\nabla_{v}^{2}V-V\nabla_{v}^{2}U)dx} = \int_{s} \nabla \cdot (U\nabla V - V\nabla U)$ reciprocity theorem, and thus signal calculations; dn points outwards Green's function method. ∂s

Green's reciprocity equation

Reciprocity is a direct consequence of the Green identities if the potentials U and V at infinity are 0:

$$\int_{S} (U\nabla^2 V - V\nabla^2 U) dx = \oint_{\partial S} (U\nabla V - V\nabla U) \cdot dn = 0$$

$$\int_{S} V \rho_U = \int_{V} U \rho_V dx$$

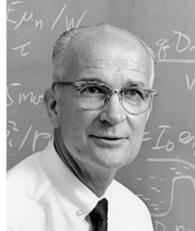
The dispersion is used to calculate the

The discrete version is used to calculate the current on electrodes, by comparison of 2 configurations:

$$\sum_{i} V_{i} q_{i}^{U} = \sum_{i} U_{i} q_{i}^{V}$$

William Bradford Shockley (1910–1989)

Configurations



Let's consider the following 2 configurations:

Wire *j*: • $V = V_j, q = q_j + \lambda_j$ Wire $i \neq j$: • $V = V_i, q = q_i + \lambda_i$ Charge: • V = ?, q = Q Wire *j*: $V = q_{j}\phi(z_{j}-z_{j}), q = q_{j}$ Wire $i \neq j$: $V = q_{j}\phi(z_{i}-z_{j}), q = 0$ Charge: $V = q_{j}\phi(z_{Q}-z_{j}), q = 0$

[W. Shockley, *Currents to Conductors Induced by a Moving Point Charge*, J. Appl. Phys. **9** (1938) 635-636. Affiliation: Bell Telephone Laboratories, NY. A closely related argument can already be found in Maxwell's *Treatise* (1873).]

Deriving the weighting field

Applying reciprocity gives: $\sum \lambda_i \phi(z_j - z_i) = -Q\phi(z_{\text{charge}} - z_j)$ Differentiating to time: $\sum_{i=1}^{n_{\text{wires}}} I_i \phi(z_j - z_i) = Q \vec{\epsilon} (z_{\text{charge}} - z_j) \cdot \vec{v}_{\text{charge}}$ $\blacktriangleright \text{ Identify } C_{ij}^{-1} = \phi(z_i - z_j) \text{ and solve for the currents:}$ $I_{i} = Q \sum \left(C_{ij} \vec{\epsilon} (z_{\text{charge}} - z_{j}) \right) \cdot \vec{v}_{\text{charge}}$ $= Q \vec{E}_{w} (z_{charge} - z_{i}) \cdot \vec{v}_{charge}$ Thus, \vec{F} is computed using columns of the capacitance matrix elements as charges.

Summary

Mechanism:

- charged particles deposit of most probably ~40 e⁻/cm;
- > the electrons move with a drift speed of 1-5 cm/ μ sec;
- \triangleright they diffuse during transport, typically 200 µm over 1 cm;
- they multiply near an electrode;
- ▶ measurement relies on recording ion $+ e^{-}$ movement.
- Electron transport is driven by inelastic collisions.
- Multiplication is not only a matter of direct ionisation, but is also influenced by excitation/de-excitation of noble gases.