Chapter 1

Diffusion

1.1 Introduction

Electrons and ions in a gas and subject only to an electric field move on average along the electric field, but individual electrons deviate from the average due to scattering on the atoms of the gas. Scattering leads to variations in velocity, called longitudinal diffusion, and to latteral displacements, called transverse diffusion. The scattering process in each direction can to a good approximation be considered Gaussian on a microscopic scale.

In the presence of both an electric and a magnetic field, the average motion has in general components parallel with E, with B_{T}, the component of B which is transverse to E, and with $E \times B$. The direction of the velocity vector is usually obtained from the Magboltz 2 program, and can also be approximated with the Laue-Langevin equation. Scattering leads, as before, to variations in velocity and to lateral displacements but due to the magnetic field, there are now 2 lateral components which need not be equal.

In view of the Gaussian nature of the diffusion process, it is natural to describe it in terms of a 3-dimensional normal distribution with the longitudinal and transverse diffusion coefficients as diagonal terms of the covariance matrix. In the absence of physical correlations between the diffusion coefficients, the covariance matrix is diagonal in a frame in which the average direction of motion is one of the axes and in which the other 2 axes are suitably chosen. In an arbitrary frame of reference, or in the presence of physical correlations, however, the covariance matrix will not be diagonal but it will still be symmetric. We therefore add a further 3 coefficients to build a (symmetric) covariance matrix which enables us to formulate the diffusion process independent of a coordinate system. The independence of a coordinate system authorises us to call this matrix the diffusion tensor.

If the E and B fields are not homogeneous, the mean drift paths from neighbouring points will diverge or converge, while particles may accelerate or decelerate along the mean drift path. Field inhomogeneities therefore modulate both the longitudinal and the transverse diffusion process caused by the gas.

1.2 Diffusion coefficients

1.2.1 Electrons

Longitudinal and transverse diffusion coefficients have been measured for a variety of pure gases and gas mixtures over a broad range of E fields. Measurements with a B field are scarce however and rarely will one find data for the exact configuration of E and B fields one needs. It has therefore become usual to rely on calculations, often with Magboltz 2, for these coefficients.

1.2.2 Ions

Diffusion of ions is a small effect and little data seems to exists [1] [2] [3]. Since moreover there seems to be no program to compute these, one often resorts to approximating the ion diffusion with the Einstein equation.

1.3 Coordinate systems

We have to use 3 different systems which we will label m, c and v:

- m: the Magboltz 2 coordinate system, in which the directions of the axes are chosen as $(E, B_\mathrm{T}, E \times B)$, with B_T the component of B which is perpendicular to E. If E and B are parallel, and also if $B = 0$, the 2nd and 3rd axes are taken to be any 2 axes perpendicular to E;
- c: the coordinate system used for computing the drift path of the particle which is either the Cartesian coordinate system (x, y, z) or a conformal mapping thereof;
- v: a coordinate system in which the direction of the drift velocity is used as first axis, complemented with any 2 axes perpendicular to the velocity vector.

To ensure these coordinate systems are related by simple rotations, they are made right-handed by taking the vector product of the first 2 components as 3rd component.

1.4 Rotations

We write R_{ab} for the rotation matrix which transforms x_b, a vector x expressed in terms of an arbitrary coordinate system b, to x_a, the same vector x but expressed in another arbitrary coordinate system a, according to the relation $x_a = R_{ab}x_b$. Since Equation (1.5.1) is valid in any coordinate system, $x^\mathrm{T}\Sigma^{-1}x$ is a scalar quantity. This implies that the transformation law for Σ^{-1} reads $\Sigma_a^{-1} = R_{ba}^\mathrm{T}\Sigma_b^{-1}R_{ba}$ or equivalenty $\Sigma_a = R_{ba}^\mathrm{T}\Sigma_b R_{ba}$.

The rotation matrices are easy to find since we know the coordinate vectors of the systems m and v with respect to c. R_{mc} is simply the matrix which has as rows the coordinate vectors of m in terms of system c. The same goes for R_{vc}. Reverse transformations are obtained by transposing, e.g. $R_{cv} = R_{vc}^\mathrm{T}$. Rotations can be chained by multiplication, e.g. $R_{mv} = R_{mc}R_{cv} = R_{mc}R_{vc}^\mathrm{T}$.

1.5 Diffusion formalism

1.5.1 Homogeneous fields

Denoting the diffusion tensor by Σ^{-1}, and assuming homogeneous E and B fields, the probability that a particle is scattered by a vector x with respect to the average direction of motion is given by:

$$P = \frac{1}{2\pi\sqrt{|\Sigma|}} \mathrm{e}^{-\frac{1}{2}x^{\mathrm{T}}\Sigma^{-1}x}$$

Σ fully describes the diffusion process. This tensor depends on E and on B, but also on the mean distance travelled by the particle during the diffusion process.

Writing the mean distance over which the particle drifts as d, the diffusion coefficients in each of the directions as σ_1, σ_2, σ_3 and the correlation coefficients as ρ_{12}, ρ_{13}, ρ_{23}, one finds the following expression for Σ:

$$\Sigma = d \begin{pmatrix} \sigma_1^2 & \rho_{12}\sigma_1\sigma_2 & \rho_{13}\sigma_1\sigma_3 \\ \rho_{12}\sigma_1\sigma_2 & \sigma_2^2 & \rho_{23}\sigma_2\sigma_3 \\ \rho_{13}\sigma_1\sigma_3 & \rho_{23}\sigma_2\sigma_3 & \sigma_3^2 \end{pmatrix}$$

This is the natural extension of a 1-dimensional diffusion process, where $\Sigma = d\sigma^2$.

1.5.2 Inhomogeneous fields

Since E and B are in general not homogeneous, we have to apply corrections for acceleration and for convergence of the drift paths. We assume that the drift paths are integrated in sufficiently small steps to be able to consider the acceleration and convergence of the drift velocity v as locally linear. In the v coordinate frame where the velocity vector is aligned with the first coordinate axis x_1, and placing the origin at the current location of the particle, this means that $v_1 = v + \alpha_1 x_1$, $v_2 = \alpha_2 x_2$ and $v_3 = \alpha_3 x_3$. A small initial offset $r(0)$ will evolve according to an equation of the type $\dot{r}_i(t) = \alpha_i r_i(t)$. Hence after a time δt, the offset will have become $f_i r(0) = \exp(\alpha_i \delta t) r(0)$ where $\alpha_i = \mathrm{d}v_i/\mathrm{d}x_i$. This approximation is only useable when the α factors are to good approximation constant over the length of a step. This is not the case in strongly divergent or convergent areas, which are frequently encountered. Hence, Garfield evaluates the f factors explicitely by integrating neighbouring drift lines over the mean length of the step being taken, for transverse locations which are 1 mean step length away from the starting point of the step. This coordinate stretch can be described by the convergence matrix F:

$$F = \begin{pmatrix} f_1 & 0 & 0 \\ 0 & f_2 & 0 \\ 0 & 0 & f_3 \end{pmatrix}$$

with the help of which the diffusion equation for non-uniform fields can be written as:

$$P = \frac{1}{2\pi\sqrt{|F\Sigma F|}} \mathrm{e}^{-\frac{1}{2}x^{\mathrm{T}}(F\Sigma F)^{-1}x}$$

The Gaussian nature of the process is not affected by acceleration and convergence, only the diffusion tensor is modified to become, what we call, the effective diffusion tensor Σ'

$$\Sigma' = F \Sigma F$$

which can also be obtained from Σ by replacing in Equation (1.5.1) σ_i by $\sigma_i \exp(f_i \delta t)$, without changing the correlation coefficients ρ_{ij}.

When tracing a particle through a fields, we do so by taking small steps each of which has its own diffusion tensor and convergence matrix. Adding steps is particularly simple thanks to the Gaussian nature of the process:

$$\Sigma'_{\text{total}} = \int F(z)\Sigma(z)F(z)\mathrm{d}z$$

1.5.3 Considerations for strongly divergent and convergent fields

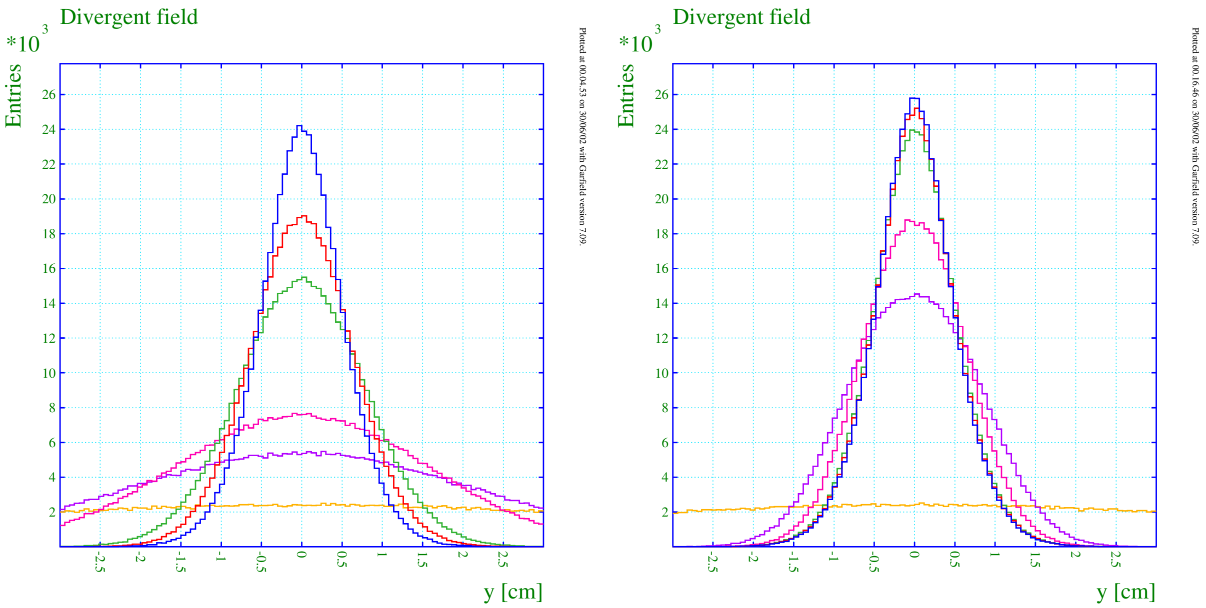

Figure 1.1: Diffusion in a strongly divergent field, in this case a purely radial field of constant magnitude, between $r = 0.01$ cm and $r = 1$ cm with $\sigma_{\mathrm{T}} = \sigma_{\mathrm{L}} = 500\ \mu\mathrm{m}$. In the left diagram, steps of constant length have been taken, while in the diagram on the right steps of constant f were used. In both cases, the number of steps is 1 (lower orange curve), 5, 10, 50, 100 and 500 (upper blue curve). Dividing into 50 steps, $f_{\max} = 2.98$ with constant length steps and $f = 1.10$ with constant f steps.

Stepping through a strongly divergent field leads to distributions of which not only the width but also the shape depends on the number of steps taken. If only a single step is taken, then one finds, necessarily, a Gaussian lateral spread. If two steps are taken, then the first will be Gaussian.

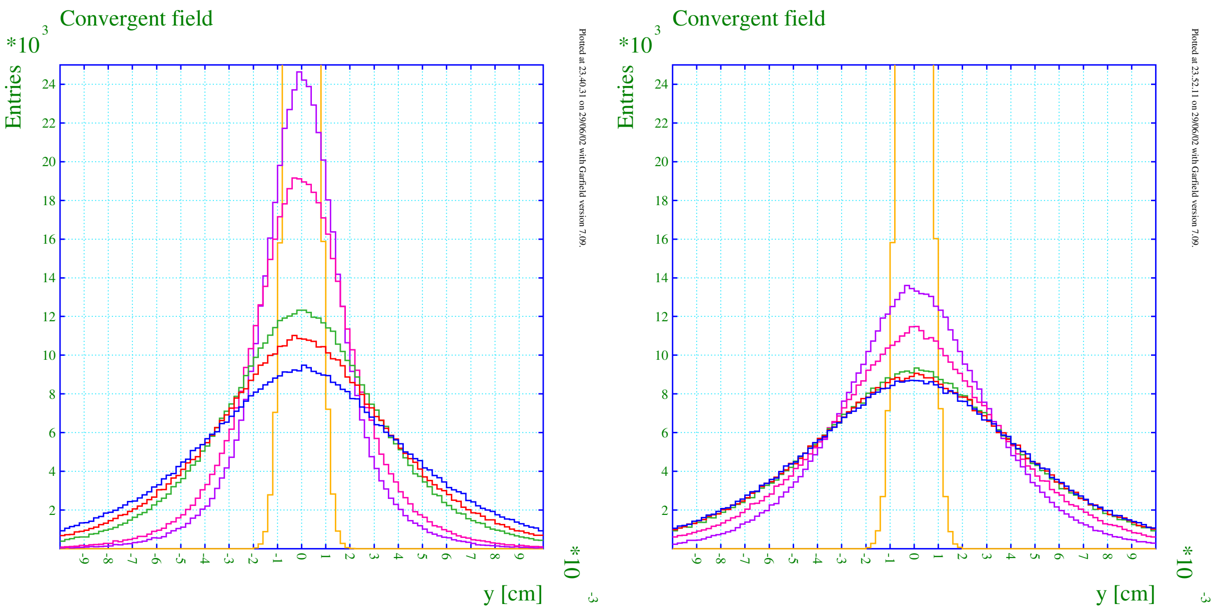

Figure 1.2: Diffusion in a strongly convergent field, in this case a purely radial field of constant magnitude, between $r = 1$ cm and $r = 0.01$ cm with $\sigma_\mathrm{T} = \sigma_\mathrm{L} = 500\ \mu\mathrm{m}$. In the left diagram, steps of constant length have been taken, while in the diagram on the right steps of constant f were used. In both cases, the number of steps is 1 (lower orange curve), 5, 10, 50, 100 and 500 (upper blue curve). Dividing into 50 steps, $f_\mathrm{min} = 0.34$ with constant length steps and $f = 0.91$ with constant f steps.

Since the field is assumed to be radial to good approximation, the second step is divergence broadened in a direction perpendicular to the first step. Hence, if the first step took the particle far transverse, the particle is likely to remain far transverse with respect to the initial direction. This may lead to a distribution with 2 pronounced peaks. One notes that the distribution narrows down considerably as more and more steps are added, see Fig. 1.5.3.

For common values of the diffusion tensor, one finds that the transverse distribution reaches its asymptotic shape to within a few percent if the largest divergence factor encoutered while taking steps f_max is less than 1.05. The asymptotic distribution is in general not Gaussian, deviations are particularly striking if the longitudinal diffusion exceeds transverse diffusion.

Similar considerations apply to strongly converging fields, see Fig. 1.5.3 In this case the width increases with the number of steps. An asymptotic form is reached within a few percent if steps are made such that $f > 0.95$.

The mean free path λ of a drifting electron in a gas with density ρ and cross section σ, given by ρ/σ, equals $0.1-10\ \mu\mathrm{m}$ in Argon based gas mixtures. The larger values applying to drift fields for which the distribution function peaks at the Ramsauer dip, if present. Values of order $1\ \mu\mathrm{m}$ are common for moderate drift fields and $0.1\ \mu\mathrm{m}$ is more typical for the large fields encountered near the read-out electrodes, which is where strongly divergent fields are found.

Although using the asymptotic distribution may imply that steps smaller than the mean free path are taken, it seems therefore appropriate, in most cases, to simulate the diffusion process with the approximation of the asymptotic distribution which is obtained by reducing the step length to ensure that $0.95 < f < 1.05$. For reasons of numerical efficiency, it is preferable to take steps at constant f rather than steps of constant length, see see Fig. 1.5.3. The permissible range of f values is under user control in Garfield. For accurate calculations, the adequacy of this setting needs to be verified on a case-by-case basis.

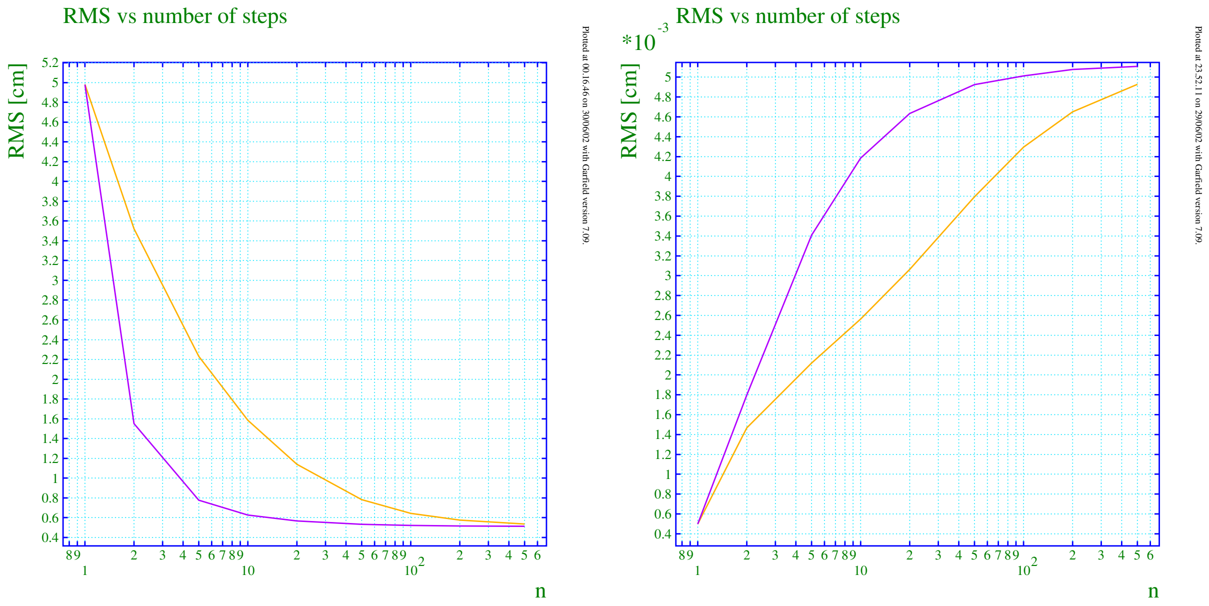

Figure 1.3: RMS of the lateral diffusion broadering in a divergent field (left) and convergent field (right). The orange curves are for equal length steps with the purple curves are for equal F steps.

1.5.4 Monte Carlo integration

Integrating the drift path by Monte Carlo proceeds along the following steps:

- compute E, B and the drift velocity v at the current location in the c frame
- compute the convergence matrix F from Equation (1.5.2) in the v frame using R_{vc}
- reduce the step size if the convergence factors are too small or too large
- interpolate the diffusion tensor Σ in the m frame and rotate Σ to the v frame using R_{vm}
- compute Σ' from Equation (1.5.2) in the v frame
- draw a random scattering vector according to Σ' and rotate the scattering vector to the c frame with R_{cv}
- update the location by adding the mean displacement, given by v and the scattering vector

- repeat the procedure unless an electrode is entered, the maximum number of steps is reached etc.

Drawing a random scattering vector according to the multivariate normal distribution given in Equation (1.5.2) is performed by first doing a Cholesky factorisation $\Sigma' = L^{\mathrm{T}} L$ where L is a lower triangular matrix. This decomposition is possible since Σ' is a positive definite symmetric matrix. Next, a 3-vector y of uncorrelated normally distributed random numbers is drawn and multiplied with L so as to obtain Ly which is distributed according to the covariance matrix Σ'.

1.5.5 Analytic integration

When diffusion is estimated after a (usually) analytic integration of the drift path, one uses Equation (1.5.2) to integrate the effective diffusion tensor over the path. This technique assumes that diffusion remains Gaussian also at the scale of a complete drift path. In the vicinity of bifurcation points, e.g. between holes of a GEM or between wires of an MWPC, this assumption is not appropriate. The method can however be useful when estimating the time spread over slightly varying drift paths leading to a single electrode, where it avoids the need of repeatedly integrating the drift path itself.

Bibliography

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