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The spatio-temporal development of electron swarms in gases: moment equation analysis and Hermite polynomial expansion z

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Abstract. **Spatio-temporal development of electron swarms in gases is simulated using a propagator method based on a series of one-dimensional spatial moment equations. When the moments up to a sufficient order are calculated, the spatial distribution function of electrons, p(x), can be constructed by an expansion technique using Hermite polynomials and the weights of the Hermite components are represented in terms of the electron diffusion coefficients. It is found that the higher order Hermite components tend to zero with time, that is, the normalized form of p(x) tends to a Gaussian distribution. A time constant of the relaxation is obtained as the ratio of the second- and third-order diffusion coefficients, D_3^2/D_L^3. The validity of an empirical approximation in time-of-flight experiments that treats p(x) as a Gaussian distribution is indicated theoretically. It is also found that the diffusion coefficient is defined as the derivative of a quantity called the cumulant which quantifies the degree of deviation of a statistical distribution from a Gaussian distribution.**

1. Introduction

The spatio-temporal development of electron swarms in gases has been analyzed in terms of a basic measurement model of electron swarm parameters such as the drift velocities and the diffusion coefficients, which are the most fundamental quantities describing the dynamics of weakly ionized plasmas and are indispensable parameters in plasma simulations based on fluid model. A history of early investigations and succeeding developments of the study on electron swarms were described by Huxley and Crompton (1974). Among the typical observation models discussed in Tagashira et al (1977), those which deal both with spatial and with temporal profiles of electron swarm evolution are

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generally called time-of-flight (TOF) experiments. Several investigations of the TOF model have been presented thereafter.

Fourier transform of the Boltzmann equation was initiated by Parker and Lowke (1969) as an analytic approach to TOF experiments, and Tagashira et al (1977) derived a solution based on a Gaussian distribution and its spatial derivatives from the eigenvalues of the Boltzmann equation. Moment (or kinetic) equation analysis is another technique by which to derive the TOF parameters (Kitamori et al 1980, Kumar 1981, Skullerud and Kuhn 1983, Skullerud 1984, Penetrante et al 1985, Robson 1991). Numerically, TOF parameters were calculated using direct estimation of moment (Kitamori et al 1980), the path integral method (Skullerud 1984), multi-term approximation of the Boltzmann equation and Monte Carlo simulation (Penetrante et al 1985), the flight-time integral method (Ikuta and Murakami 1987, Ikuta et al 1988, Robson 1995, Kumar 1995), and so forth. On the basis of the TOF method and its modified model of arrival time spectra, which was proposed by Kondo and Tagashira (1990) and Date et al (1992) to follow a practical method of experimental measurements, Nakamura (1987, 1988), Kurachi and Nakamura (1991), Hasegawa et al (1996) and Yoshida et al (1996) measured the electron drift velocities and the diffusion coefficients in N_2, CO, CO_2, SiH_4/Kr, SF_6 and CH_4.

In TOF experiments, the spatial distribution of electrons along the electric field is often approximated as a Gaussian distribution (Nakamura 1987). The drift velocity and the diffusion coefficient are derived from the temporal variations of the position of the center of mass and the variance of the distribution. This approximation seems empirically natural and appropriate, because a Gaussian distribution is the analytic solution of the second-order diffusion equation and continuity equation analyses including the terms up to the second-order gradient of the electron number density are usually adequate. However, the formal description of electron swarm development in hydrodynamic regime includes higher order terms of the density gradient (Kumar et al 1980, Pitchford et al 1981, Kumar 1981, Blevin and Fletcher 1984, Penetrante et al 1985, Robson 1991). In order to validate the approximation, which treats the spatial distribution as a Gaussian distribution, it is important to evaluate the effects of the higher order terms. At the same time, knowledge of the terms would enable us to extract their inconspicuous but present effects from practical swarm experiments.

In the present paper, the spatial moments are calculated by a propagator method (Sugawara et al 1997) based on a series of simultaneous moment equations. An expansion technique using Hermite polynomials is introduced to derive the spatial distribution of electrons from the spatial moments. The weights of the Hermite components, which are represented as functions of the higher order diffusion coefficients, and their time dependence are evaluated quantitatively in order to determine why consideration of the terms up to the second order are effectively sufficient in continuity equation analyses; and why and when the spatial distribution of electrons can be

approximated as a Gaussian distribution.

2. Calculation method

2.1. Moment equations

The spatio-temporal development of an electron swarm under a uniform electric field $E = (E_x; 0; 0)$ applied in the x direction is considered here. Generally, the term `moment' indicates both of the spatial and velocity moments; however, it implies the spatial moment with respect to the x direction in the present paper, hereafter.

The nth-order moment m_n is obtained from the electron distribution function $f(r; v; t)$ defined in the phase space $(r; v) = (x; y; z; v_x; v_y; v_z)$ as

$$m_n(t) = \int_{r;v} x^n f(r; v; t) dr dv. \tag{1}$$

The values of m_0, m_1 and m_2 are related to some basic statistical quantities, namely the electron population, the centroid (the mean position) and the variance of an electron swarm.

The moment equations, which represent the temporal variation of m_n, are derived from the Boltzmann equation by integrating it with the weight of x^n as

$$\int_r x^n \frac{\partial}{\partial t} f(r; v; t) dr = \int_r x^n \left(-a \cdot \frac{\partial}{\partial v} - v \cdot \frac{\partial}{\partial r} + \frac{\partial}{\partial t} \right)_{coll} f(r; v; t) dr \tag{2}$$

$$\frac{\partial}{\partial t} m_n(v; t) = -a_x \frac{\partial}{\partial v_x} m_n(v; t) + n v_x m_{n-1}(v; t) + \left(\frac{\partial}{\partial t} \right)_{coll} m_n(v; t) \tag{3}$$

where $a = (a_x; 0; 0) = (eE_x/m; 0; 0)$ is the acceleration due to E, e and m are the electronic charge and mass, and the subscript `coll' represents the collision term. Equation (3) shows that the moment equations have a system of hierarchy and they can be calculated in velocity space.

2.2. The propagator method

The propagator method is a calculation technique by which to obtain the electron distribution in phase space. Phase space is divided into small sections called cells and the electron motion between cells due to drift and collision processes is calculated using a function called the propagator. Sugawara et al (1997) performed a simultaneous calculation of zeroth and first-order moment equations to obtain the centroid drift velocity of electron swarms. This technique is extended for multi-order moment equations in the present paper.

In the present model, the moment equations can be calculated in two-dimensional velocity space $(v) = (v; \theta)$ due to the rotational symmetry of $f(v; \theta)$ around v_x axis.

Velocity space (v; í) is divided into cells prepared for every Åè and Åí as shown in ågure 1, in which è is the electron energy corresponding to the electron velocity v.

Since the electrons in a cell dv have a coherent velocity, they move together and their spatial motion appears as a parallel shift during a short period Åt of collisionless çight. When the initial values of m_n are known, the values after the çight of distance Åx are obtained as follows:

$$m_n(v;t) = \int_{-1}^{1} x^n p(x;v;t)dx \tag{4}$$

$$m_n(v;t+\Delta t) = \int_{-1}^{1} x^n p(x;v;t+\Delta t)dx = \int_{-1}^{1} x^n p(x-\Delta x;v;t)dx$$

$$= \int_{-1}^{1} (x+\Delta x)^n p(x;v;t)dx = \sum_{k=0}^{n} {}_nC_k \Delta x^{n-k} m_k(v;t) \tag{5}$$

where p is the spatial distribution function of electrons, and ${}_nC_k$ represents the binomial coeécients. This calculation can be carried out leaving p unknown. Here, Åx could be evaluated as $\Delta x = v_x \Delta t$ or $\Delta x = \Delta\varepsilon/(eE_x)$ even in velocity space. The latter is adopted in the present calculation in order to satisfy the law of energy conservation in the drift motion.

A computational cell is prepared for every dv and every order n. Iterative calculation starts with appropriate initial conditions of $m_n(v)$. The drift and collision processes are alternately calculated every Åt following the development of $m_n(v)$. Practical simulation conditions will be presented in section 4.

2.3. Hermite polynomial expansion

The nth-order Hermite polynomial $H_n(X)$ is the solution of a diãerential equation $Y'' - 2XY' + 2nY = 0$. The series of $H_n(X)$ can be generated in the following way:

$$H_0(X) = 1; \quad H_1(X) = \sqrt{2}X; \quad H_{n+1}(X) = \sqrt{2}X H_n(X) - nH_{n-1}(X): \tag{6}$$

$H_n(X)$ satisåes the following orthogonality:

$$\int_{-1}^{1} H_n(X)H_m(X)\exp\left(-X^2\right)dX = \delta_{nm} n!\sqrt{\pi} \tag{7}$$

where δ_{nm} is Kronecker's delta which equals unity when n = m; otherwise it is zero.

Here, we expect that the spatial distribution of electrons, p(x), can be expanded using Hermite components deåned as $H_n(X)\exp(-X^2)$. Skullerud (1984) and Viehland (1994) applied the Hermite polynomial expansion to the electron velocity distribution. In the present case, the expansion technique is applied to the spatial distribution p(x), instead. Conditions which allow the expansion are the orthogonality shown in equation (7) and a boundary condition that $H_n(X)\exp(-X^2) \to 0$ when $X \to -1$ similarly to the expansion of the velocity distribution. Forms of some årst $H_n(X)\exp(-X^2)$ are shown in ågure 2. The zeroth order components have a Gaussian distribution.

It is important to note that X must be a dimensionless quantity since $H_n(X)$ is the sum of different orders of powers of X. In order to describe p(x) using $H_n(X)$, the following dimensionless quantities are defined upon introducing the unit length $\sqrt{2}\sigma$; namely the length X, the spatial distribution P(X) and the n-th order moment M_n:

$$X = \frac{x}{\sqrt{2}\sigma} \tag{8}$$

$$P(X) = p(x)\frac{dx}{dX} = \sqrt{2}\sigma p(x) \tag{9}$$

$$M_n = \int_{-1}^{1} X^n P(X)dX = \left\{\frac{m_n}{\sqrt{2}\sigma}\right\}_n \tag{10}$$

where σ is the standard deviation of p(x) defined as $\sigma^2 = (m_2/m_0) - (m_1/m_0)^2$, which is time-dependent. Then P(X) and p(x) are expanded as

$$P(X) = \sum_{n=0}^{\infty} P_n(X) = \sum_{n=0}^{\infty} C_n H_n(X)\exp(-X^2) \tag{11}$$

$$p(x) = \sum_{n=0}^{\infty} p_n(x) = \frac{1}{\sqrt{2}\sigma}\sum_{n=0}^{\infty} C_n H_n\left(\frac{x}{\sqrt{2}\sigma}\right)\exp\left(-\frac{x^2}{2\sigma^2}\right) : \tag{12}$$

Here, C_n is a constant which represents the weight of the nth-order Hermite component. The factor $\sqrt{2}$ of the unit length appears so that $C_n = 0$ $(n \neq 1)$ when p(x) itself is a Gaussian distribution.

Considering equations (7) and (10), C_n is given by the following equation:

$$C_n n!\sqrt{2}\sigma = \int_{-1}^{1} H_n(X)P(X)dX = \sum_{k=0}^{n} S_{n;k}M_k \tag{13}$$

$$S_{n;k} = (-1)^{(n-k)/2}\left\{\sqrt{2}\right\}_{2k-n}\frac{n!}{\{(n-k)/2\}!k!} \tag{14}$$

where $S_{n;k}$ $(n \geq k \geq 0)$ is the coefficient of X^k in $H_n(X)$, and $n - k$ must be an even integer, otherwise $S_{n;k} = 0$. Some first C_n are obtained as follows:

$$C_0 = \frac{M_0}{0!\sqrt{2}\sigma} = \frac{1}{0!\sqrt{2}\sigma}m_0 \tag{15}$$

$$C_1 = \frac{\sqrt{2}M_1}{1!\sqrt{2}\sigma} = \frac{1}{1!\sqrt{2}\sigma}\frac{m_1}{\sigma} \tag{16}$$

$$C_2 = \frac{2M_2 - M_0}{2!\sqrt{2}\sigma} = \frac{1}{2!\sqrt{2}\sigma}\left(\frac{m_2}{\sigma^2} - m_0\right) \tag{17}$$

$$C_3 = \frac{2\sqrt{2}M_3 - 3\sqrt{2}M_1}{3!\sqrt{2}\sigma} = \frac{1}{3!\sqrt{2}\sigma}\left(\frac{m_3}{\sigma^3} - 3\frac{m_1}{\sigma}\right) \tag{18}$$

$$C_4 = \frac{4M_4 - 12M_2 + 3M_0}{4!\sqrt{2}\sigma} = \frac{1}{4!\sqrt{2}\sigma}\left(\frac{m_4}{\sigma^4} - 6\frac{m_2}{\sigma^2} + 3m_0\right) \tag{19}$$

$$C_5 = \frac{4\sqrt{2}M_5 - 20\sqrt{2}M_3 + 15\sqrt{2}M_1}{5!\sqrt{2}\sigma} = \frac{1}{5!\sqrt{2}\sigma}\left(\frac{m_5}{\sigma^5} - 10\frac{m_3}{\sigma^3} + 15\frac{m_1}{\sigma}\right) : \tag{20}$$

When m_n is represented as the central moment relative to the centroid of $p(x)$, the fastest convergence with respect to n will be expected. Coordinates can be easily converted from a laboratory system to the centroid system using equation (5). We obtain $m_1 = 0$ and $\sigma^2 = m_2/m_0$ in the centroid system; therefore, always $C_1 = C_2 = 0$.

Note here that the electron motion is calculated by using the moment equations independently of the Hermite expansion technique, which is applied only to construct $p(x)$ at a moment based on the instantaneous values of m_n, in contrast to the fact that other conventional expansion techniques using Fourier transform and Legendre polynomials are applied to describe the electron motion in real space and velocity space.

3. Relation between physical and statistical quantities

3.1. The spatial moments and the diffusion coefficients

An interesting fact is that the normalized weights C_n/m_0 of Hermite components of $p(x)$ are represented in terms of the higher order electron diffusion coefficients D_n mediated by the spatial moments m_n. D_n are defined as the coefficients of the spatial gradient terms of the electron number density in the electron continuity equation below:

$$\frac{\partial}{\partial t}p(x;t) = \left[R_i - W_r\frac{\partial}{\partial x} + D_L\frac{\partial^2}{\partial x^2} - D_3\frac{\partial^3}{\partial x^3} + D_4\frac{\partial^4}{\partial x^4} - \cdots \right] p(x;t) \tag{21}$$

where R_i is the ionization frequency, W_r is the centroid drift velocity and D_L ($= D_2$) is the second-order longitudinal diffusion coefficient. D_n are derived as shown below from equation (21) by integrating it with the weight $(x - g)^n$, where g is the centroid of $p(x)$:

$$D_n = \frac{1}{n!}\frac{d}{dt}\int_{-1}^{1}(x-g)^n\frac{p(x;t)}{m_0}dx - \sum_{k=2}^{n}\frac{1}{(n-k)!}D_k\int_{-1}^{1}(x-g)^{n-k}\frac{p(x;t)}{m_0}dx \tag{22}$$

$$= \frac{1}{n!}\frac{d}{dt}\frac{m_n}{m_0} - \sum_{k=2}^{n}\frac{1}{(n-k)!}D_k\frac{m_{n-k}}{m_0}. \tag{23}$$

The early derivation of D_n presented as equation (5) by Tagashira et al (1977) includes an extra factor $(-1)^k$. However, according to the present verification, this factor seems unnecessary when the right-hand side of equation (21) originally has alternate negative signs. A practical difference in D_n due to $(-1)^k$ term appears for $n \geq 5$, thus, the definitions of D_L, D_3 and D_4 are common to both equations.

One can rewrite C_n/m_0 by appropriately replacing the moments in equations (15){(20) with D_n based on the results of recursive transformations of D_n using equation (23).

C_n/m_0 are constants for $n = 0; 1; 2$:

$$\frac{C_0}{m_0} = \frac{1}{\sqrt{2\pi}\sigma}; \quad \frac{C_1}{m_0} = \frac{1}{\sqrt{2\pi}\sigma}\frac{m_1}{\sigma} = 0; \quad \frac{C_2}{m_0} = \frac{1}{2!\sqrt{2\pi}\sigma}\frac{m_2 - \sigma^2}{\sigma^2} = 0. \tag{24}$$

For $n = 3; 4; 5$, each $C_n=m_0$ is represented by a corresponding D_n respectively

$$\frac{C_3}{m_0} = \frac{3!D_3t + m_{3;0}}{3!\sqrt{\pi}(2!D_Lt + m_{2;0})^{3=2}} = \frac{\hat{\imath}_3}{3!\sqrt{\pi}\,\hat{\imath}_2^{3=2}} \tag{25}$$

$$\frac{C_4}{m_0} = \frac{4!D_4t + m_{4;0}}{4!\sqrt{\pi}(2!D_Lt + m_{2;0})^{4=2}} = \frac{\hat{\imath}_4}{4!\sqrt{\pi}\,\hat{\imath}_2^{4=2}} \tag{26}$$

$$\frac{C_5}{m_0} = \frac{5!D_5t + m_{5;0}}{5!\sqrt{\pi}(2!D_Lt + m_{2;0})^{5=2}} = \frac{\hat{\imath}_5}{5!\sqrt{\pi}\,\hat{\imath}_2^{5=2}} \tag{27}$$

where $\hat{\imath}_n = n!D_nt + m_{n;0}$ is obtained from integration of D_n with respect to time and $m_{n;0}$ is a constant which appears in the integration.

For $n \geq 6$, additional terms other than $\hat{\imath}_n$ appear in the representation of $C_n=m_0$:

$$\frac{C_6}{m_0} = \frac{\hat{\imath}_6 + 10\,\hat{\imath}_3^2}{6!\sqrt{\pi}\,\hat{\imath}_2^{6=2}} \tag{28}$$

$$\frac{C_7}{m_0} = \frac{\hat{\imath}_7 + 35\,\hat{\imath}_4\,\hat{\imath}_3}{7!\sqrt{\pi}\,\hat{\imath}_2^{7=2}} \tag{29}$$

$$\frac{C_8}{m_0} = \frac{\hat{\imath}_8 + 56\,\hat{\imath}_5\,\hat{\imath}_3 + 35\,\hat{\imath}_4^2}{8!\sqrt{\pi}\,\hat{\imath}_2^{8=2}} \tag{30}$$

$$\frac{C_9}{m_0} = \frac{\hat{\imath}_9 + 84\,\hat{\imath}_6\,\hat{\imath}_3 + 126\,\hat{\imath}_5\,\hat{\imath}_4 + 280\,\hat{\imath}_3^3}{9!\sqrt{\pi}\,\hat{\imath}_2^{9=2}}: \tag{31}$$

The numerators in these equations consist of $\hat{\imath}_i$ satisfying $i \geq 3$, the sum of the subscripts i in a term is n, and any combination of such subscripts appears in the numerators.

Considering that each $\hat{\imath}_n$ is a linear function with respect to t under an assumption that D_n is a constant in equilibrium, comparison of the orders of t in each pair of numerator and denominator of $C_n=m_0$ gives a result that $C_n=m_0$ $(n \geq 3)$ tend to zero when $t \to \infty$. This result indicates that the normalized form of $p(x)$ tends to a Gaussian distribution.

3.2. The diffusion coefficients and the cumulants

In fact, $\hat{\imath}_n$ is a statistical quantity called the cumulant. The relation between the electron diffusion coefficients and the cumulants is presented in this subsection.

Introducing a parameter $\hat{u}$, the moment generating function $M(\hat{u})$ for the moment m_n and the cumulant generating function $K(\hat{u})$ for the cumulant $\hat{\imath}_n$ are defined formally as follows:

$$M(\hat{u}) = \sum_{n=0}^{\infty} m_n \frac{\hat{u}^n}{n!} = \int_{-\infty}^{\infty} \exp(\hat{u}x)p(x)dx \tag{32}$$

$$K(\hat{u}) = \sum_{n=1}^{\infty} \hat{\imath}_n \frac{\hat{u}^n}{n!} = \log \frac{M(\hat{u})}{m_0} \tag{33}$$

where $M(\hat{u})$ has been divided by m_0 in equation (33), in order to treat $\hat{\imath}_n$ as normalized values. It is known that $\hat{\imath}_n = 0$ $(n \geq 3)$ when $p(x)$ is a Gaussian distribution; thus the cumulants are recognized as quantities representing the degree of deviation of $p(x)$ from a Gaussian distribution.

A kind of continuity equation of $M(\hat{u})$ is obtained as follows by integrating equation (21) with the weight of $\exp(\hat{u}x)$:

$$\frac{\partial}{\partial t} M(\hat{u}) = \left\{ R_i + W_r \hat{u} + D_L \hat{u}^2 + D_3 \hat{u}^3 + \cdots \right\} M(\hat{u}) \tag{34}$$

where the operators $(\partial^n/\partial x^n)$ have been replaced with $(-1)^n \hat{u}^n$ in n times of partial integrations. Using the relation $M(\hat{u}) = m_0 \exp\{K(\hat{u})\}$ derived from equation (33), equation (34) is rewritten as

$$R_i + W_r \hat{u} + D_L \hat{u}^2 + D_3 \hat{u}^3 + \cdots = \frac{\partial M(\hat{u})/\partial t}{M(\hat{u})} = \frac{(\partial/\partial t) m_0 \exp\{K(\hat{u})\}}{m_0 \exp\{K(\hat{u})\}} \tag{35}$$

$$= \frac{1}{m_0}\frac{dm_0}{dt} + \frac{\partial}{\partial t}\left(\hat{\imath}_1 \hat{u} + \frac{1}{2!}\hat{\imath}_2 \hat{u}^2 + \frac{1}{3!}\hat{\imath}_3 \hat{u}^3 + \cdots \right). \tag{36}$$

A comparison of the coefficients of $\hat{u}$ gives the following relation:

$$D_n = \frac{1}{n!}\frac{d}{dt}\hat{\imath}_n \quad (n \geq 2). \tag{37}$$

Conventionally, D_n have been considered as the derivatives of m_n. However, the physical meaning of the second term in equation (23) has never been explained clearly. Now D_n have been proven to be the derivatives of the cumulants.

The third- and fourth-order cumulants normalized with respect to the standard deviation σ, $\hat{\imath}_3/\sigma^3$ and $\hat{\imath}_4/\sigma^4$, have been recognized to be the statistical quantities called skewness and kurtosis, respectively, which represent the degrees of asymmetry and concentration of the form of a distribution function. Effects of the skewness and the kurtosis on transport coefficients defined in real space and velocity space were discussed in Kumar et al (1980) and Viehland (1994), respectively. Equation (37) represents the relation of D_3 and D_4 to the skewness and kurtosis of a spatial distribution explicitly.

3.3. The weights of Hermite components and the cumulants

Now we know what $\hat{\imath}_n$ is. Equations (24)–(31) can be derived more analytically.

$M(\hat{u})$ is represented using the Hermite components by expanding $p(x)$ as

$$M(\hat{u}) = \int_{-\infty}^{\infty} \exp\left\{ \sqrt{2}\sigma\hat{u}X \right\} \left(\sum_{n=0} C_n H_n(X) \exp(-X^2) \right) dX. \tag{38}$$

$$= \int_{-\infty}^{\infty} \exp\left\{ \frac{\sigma^2\hat{u}^2}{2} \right\} \left(\sum_{n=0} H_n(X) \frac{(\sigma\hat{u})^n}{n!} \right) \left(\sum_{n=0} C_n H_n(X) \exp(-X^2) \right) dX \tag{39}$$

$$= \exp\left\{ \frac{\sigma^2\hat{u}^2}{2} \right\} \sum_{n=0} n! \sqrt{\pi}\, C_n \frac{(\sigma\hat{u})^n}{n!} \tag{40}$$

where the quantity $\exp\left[\frac{1}{2}\sigma\hat{\omega}X\right]$ in equation (38) has been rewritten using the generating function of Hermite polynomials. Equation (40) becomes

$$\sum_{n=0}\frac{C_n}{m_0}(\sigma\hat{\omega})^n = \frac{1}{\sqrt{\sigma}}\exp\left[-\frac{\sigma^2\hat{\omega}^2}{2}\right]\exp\{K(\hat{\omega})\} \tag{41}$$

$$= \frac{1}{\sqrt{\sigma}}\exp\left[-\frac{1}{2}\sigma^2\hat{\omega}^2 + \hat{\iota}_1\hat{\omega} + \frac{1}{2!}\hat{\iota}_2\hat{\omega}^2 + \frac{1}{3!}\hat{\iota}_3\hat{\omega}^3 + \cdots\right]. \tag{42}$$

Again, a comparison of the coefficients of $\hat{\omega}$ gives the relations between C_n and $\hat{\iota}_n$. We obtain $\hat{\iota}_1 = 0$ and $\hat{\iota}_2 = \sigma^2$ since $C_1 = C_2 = 0$; therefore

$$\sum_{n=0}\frac{C_n}{m_0}(\sigma\hat{\omega})^n = \frac{1}{\sqrt{\sigma}}\exp\left[\sum_{i=3}\frac{1}{i!}\hat{\iota}_i\hat{\omega}^i\right] = \frac{1}{\sqrt{\sigma}}\prod_{i=3}\left\{\sum_{j=0}\frac{1}{j!}\left[\frac{1}{i!}\hat{\iota}_i\hat{\omega}^i\right]^j\right\}. \tag{43}$$

It has been analytically shown here why the numerators in equations (28){(31) consist of $\hat{\iota}_i$ satisfying $i \geq 3$, why the sum of the subscripts i in a term is n and why any combination of such subscripts appears in the numerators.

4. Simulation conditions

The development of an electron swarm in SF_6 at E=N of 1414 Td (E = 500 V cm^{-1} at 1 Torr, 0°C) is simulated. The number density of gas molecules N at 0°C is $3{:}54\times10^{16}$ cm^{-3}. Here, SF_6 is chosen as an example of real gases. SF_6 involves varieties of electron collision processes such as ionization, electron attachment, vibrational and electronic state excitations as well as elastic collision. The set of the electron collision cross sections of SF_6 is taken from Itoh et al (1993), which has been prepared well so that one can reproduce experimental data of the diffusion coefficients as well as the ionization coefficient and the drift velocity. Computationally, SF_6 is more complicated than rare gases because of the collision processes; however, the relaxation of the electron energy distribution is far faster with it.

It is assumed that the initial electrons start from x = 0 with the Maxwellian velocity distribution with a mean energy of 1 eV. The moments from m_0 up to m_9 are calculated here simultaneously. The cell widths and the time step for the propagator method are determined to be $\Delta\varepsilon = 0{:}2$ eV, $\Delta x = \hat{\sigma}/90$ rad and $\Delta t = 0{:}1$ ps. In order to verify the results of the propagator method, a Monte Carlo simulation is performed under the same condition.

5. Results and discussion

5.1. The spatio-temporal development of an electron swarm

Figure 3 is the calculation result of p(x; t) of an electron swarm. Equilibrium values of the mean energy $\bar{\varepsilon}$ and other electron swarm parameters obtained by the two methods

are listed in table 1. As an unavoidable tendency in numerical calculation, the instability of the calculation results increases with the increase in the order of the electron swarm parameters. The value of D_4 by the Monte Carlo simulation is reliable only in its order of magnitude, since the statistical çuctuation of the higher order moments was large even though two million electrons were sampled in the simulation. However, the two results agree well with each other, that veriåes the principle of the present moment equations and propagator method.

Table 1. **Electron swarm parameters calculated by a Monte Carlo simulation (MC) and a propagator method (PM) in SF_6 at E=N = 1414 Td.**

Method	ẽ (eV)	R_i ($s^{Ä1}$)	W_r (cm $s^{Ä1}$)	D_L (cm^2 $s^{Ä1}$)	D_3 (cm^3 $s^{Ä1}$)	D_4 (cm^4 $s^{Ä1}$)
MC	**14:88**	**514:2 Ç 10^6**	**68:1 Ç 10^6**	**0:945 Ç 10^6**	**5:56 Ç 10^3**	**Ä16:7**
PM	**14:89**	**514:3 Ç 10^6**	**68:2 Ç 10^6**	**0:957 Ç 10^6**	**6:02 Ç 10^3**	**Ä11:8**

Figure 4 shows how p(x) is constructed by the Hermite components. In order to demonstrate the contribution of the higher order components to p(x), an asymmetric p(x) has been chosen here. Since an early distribution form has a strong asymmetry, a part of p(x) is numerically negative. However, this simply indicates that more components are required to express p(x) precisely when p(x) is asymmetric. Nonetheless, it has been demonstrated that a primary portrait can be reproduced by some årst few orders of Hermite components.

5.2. The electron energy distribution

The electron energy distribution, F(è), at t = 4 ns calculated from $m_0(v; î)$ is shown in ågure 5. It has been conårmed that electron swarm parameters deåned in velocity space, such as the mean energy and the average velocity, had reached their equilibrium values by this moment.

As indicated by the large population of high-energy electrons in ågure 5, as well as by the large R_i in table 1, ionization (threshold $è_{ion}$ = 15:8 eV) occurs frequently under this condition. One may suspect that ionization may deform the Gaussian form of the spatial distribution since high-energy electrons tend to locate themselves within the leading part of an electron swarm. In order to examine this point, the energy-resolved spatial distribution of electrons is presented in ågure 6, which is constructed in the same way as ågure 3 by applying the Hermite expansion technique to the energy-resolved moments. It is true that the centroid of high energy electrons is shifted forward from that of the entire electron swarm. However, the electrons with energies higher than $è_{ion}$ are distributed almost throughout the entire range of the swarm, keeping their forms

close to Gaussian distributions. Ionization does not seem to deform the Gaussian profile of p(x).

5.3. The relaxation time

Figure 7 shows the temporal variations of the cumulants $\hat{\imath}_2$ (= m_2) and $\hat{\imath}_3$ (= m_3). The effect of the first stage of electron swarm development, relaxation of F(è), appears as $m_{2;0}$ and $m_{3;0}$, and this stage is less than 1 ns. Figure 8 shows the temporal decay of C_n/m_0 ($n \geq 3$), that confirms the convergence of p(x) to a Gaussian distribution. This process is the second stage.

The order of t in the representations of C_n/m_0 gives an index of its speed of asymptotic decay. This order is denoted as O_n (< 0) hereafter, and the most significant order, which is closest to zero, is adopted as O_n when C_n/m_0 has terms with different orders. We obtain $O_n = [n/3] - n/2$, where [x] is Gauss' truncation symbol which represents the greatest integer that does not exceed x. O_n is closest to zero at n = 3, for which the speed of decay is slowest. While $-n/2$ decreases linearly, [n/3] increases in a stepwise manner for every increment of three in n due to the rule `C_n/m_0 consists of $\hat{\imath}_i$ ($i \geq 3$)'. O_n takes maximum values when n is a multiple of three due to the factor $\hat{\imath}_3^{n/3}$, and its influence appears in figure 8 as slow decay of C_3, C_6 and C_9.

One can treat p(x) as a Gaussian distribution when the most significant coefficient C_3/m_0 is small enough. The lifetime of C_3/m_0 can be evaluated by a kind of time constant $\tau = D_3^2/D_L^3$ derived from the coefficient part of t in C_3/m_0 by omitting the constant factors. $\tau/t \geq 1$ is a criterion for the approximation. The time dependence $t^{-1/2}$ of the third-order coefficient agrees with a prediction by Kumar et al (1980, section 2). Here, τ = 0.04 ns under the present condition at 1 Torr and other examples of τ calculated by Date et al (1992) for Kr at E/N = 200 Td and 500 Td at 1 Torr were around 0.3 ns.

The relaxation time of an electron swarm depends on E/N and it is in inverse proportion to the gas pressure at a practical value of E/N. The order of magnitude of the delay time, converted to that at 1 Torr, for a measurement shot is from 100 ns to 1 ìs or more (Nakamura 1987, 1988, Yoshida et al 1996, Shishikura et al 1997). Although the decay of a function of t^{-n} type is generally much slower than that of an exponential decay, both of the first and second stages of the electron swarm development will finish by the moment of observation in practical electron swarm experiments.

5.4. Treatment in continuity equation analyses

The effect of the higher order diffusion coefficients on p(x) diminishes and p(x) tends to a Gaussian distribution which is the analytic solution of the second-order diffusion equation with constant transport coefficients. A continuity equation is identical to

a diffusion equation with constant transport coefficients when $F(\varepsilon)$ is in equilibrium everywhere under a uniform electric field.

In most of conventional continuity equation analyses, the electron number density gradient terms up to the second order are calculated and the higher order diffusion terms other than the usual second-order one are rarely considered. The reason why one can adopt this treatment without incurring a considerable error seems to be not simply because the higher order transport coefficients are regarded as being small, but rather because the effect of the higher order terms diminishes in any case. Convergence of p(x) to a Gaussian distribution would be a theoretical explanation for the empirical approximation.

6. Conclusions

The spatio-temporal development of electron swarms in gases under a uniform electric field was described by simultaneous spatial moment equations. The spatial distribution of electrons can be constructed using a Hermite polynomial expansion technique based on the spatial moments calculated by a propagator method. The present calculation result agreed well with that of a Monte Carlo simulation. The relaxation process of electron swarms includes two successive stages, namely relaxations of the electron energy distribution and the form of the spatial distribution.

The weights of the Hermite components are represented in terms of the higher order electron diffusion coefficients, for which a more substantial definition as the derivatives of statistical quantities called cumulants has been given. The representations of the weights indicate that the normalized form of the spatial distribution of electrons converges to a Gaussian distribution, as is empirically approximated in time-of-flight experiments. The speed of convergence of the spatial distribution of electrons to a Gaussian distribution is dominated primarily by the second- and third-order diffusion coefficients, D_L and D_3. A time constant D_3^2/D_L^3 was derived to evaluate the relaxation time necessary to attain a Gaussian distribution.

The effect of higher order diffusion coefficients disappears in long-time solution of the spatio-temporal development of an electron swarm. This result indicates that a standard treatment in continuity equation analyses taking into account of the density gradient terms up to the second order, namely the usual diffusion term, and truncating the other higher order terms seems reasonable not only on empirical grounds but also on the theoretical grounds.

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References

Blevin H A and Fletcher J 1984 Aust.J.Phys. 37 **593-600**
Date H, Kondo K, Yachi S and Tagashira H 1992 J. Phys. D: Appl. Phys. 25 **1330-4**
Hasegawa H, Date H, Shimozuma M, Yoshida K and Tagashira H 1996 J. Phys. D: Appl. Phys. 29 **2664-7**
Huxley L G H and Crompton R W 1974 The Diãusion and Drift of Electrons in Gases **(Wiley, New York)**
Ikuta N and Murakami Y 1987 J.Phys.Soc.Jpn. 56 **115-27**
Ikuta N, Takeda A and Yamamoto K 1988 J.Phys.Soc.Jpn. 57 **2401-15**
Itoh H, Matsumura T, Satoh K, Date H, Nakao Y and Tagashira H 1993 J. Phys. D: Appl. Phys. 26 **1975-9**
Kitamori K, Tagashira H and Sakai Y 1980 J. Phys. D: Appl. Phys. 13 **535-50**
Kondo K and Tagashira H 1990 J. Phys. D: Appl. Phys. 23 **1175-83**
Kumar K, Skullerud H R and Robson R E 1980 Aust.J.Phys. 33 **343-448**
Kumar K 1981 J. Phys. D: Appl. Phys. 14 **2199-208**
Kumar K 1995 J.Phys.Soc.Jpn. 64 **4583-8**
Kurachi M and Nakamura Y 1991 IEEE Trans. Plasma Sci. 19 **262-9**
Nakamura Y 1987 J. Phys. D: Appl. Phys. 20 **933-8**
| | 1988 J. Phys. D: Appl. Phys. 21 **67-72**
Parker J H Jr and Lowke J J 1969 Phys. Rev. 181 **290-301**
Penetrante B M, Bardsley J N and Pitchford L C 1985 J. Phys. D: Appl. Phys. 18 **1087-100**
Pitchford L C, O'Neil S V and Rumble J R Jr 1981 Phys. Rev. A 23 **294-304**
Robson R E 1991 Aust.J.Phys. 44 **685-92**
Robson R E 1995 Aust.J.Phys. 48 **677-89**
Shishikura Y, Asano K and Nakamura Y 1997 J. Phys. D: Appl. Phys. 30 **1610-5**
Skullerud H R and Kuhn S 1983 J. Phys. D: Appl. Phys. 16 **1225-34**
Skullerud H R 1984 J. Phys. B: At. Mol. Phys. 17 **913-29**
Sugawara H, Tagashira H and Sakai Y 1997 J. Phys. D: Appl. Phys. 30 **368-73**
Tagashira H, Sakai Y and Sakamoto S 1977 J. Phys. D: Appl. Phys. 10 **1051-63**
Viehland L A 1994 Chem.Phys. 179 **71-92**
Yoshida K, Ohshima T, Ohmori Y, Ohuchi H and Tagashira H 1996 J. Phys. D: Appl. Phys. 29 **1209-16**

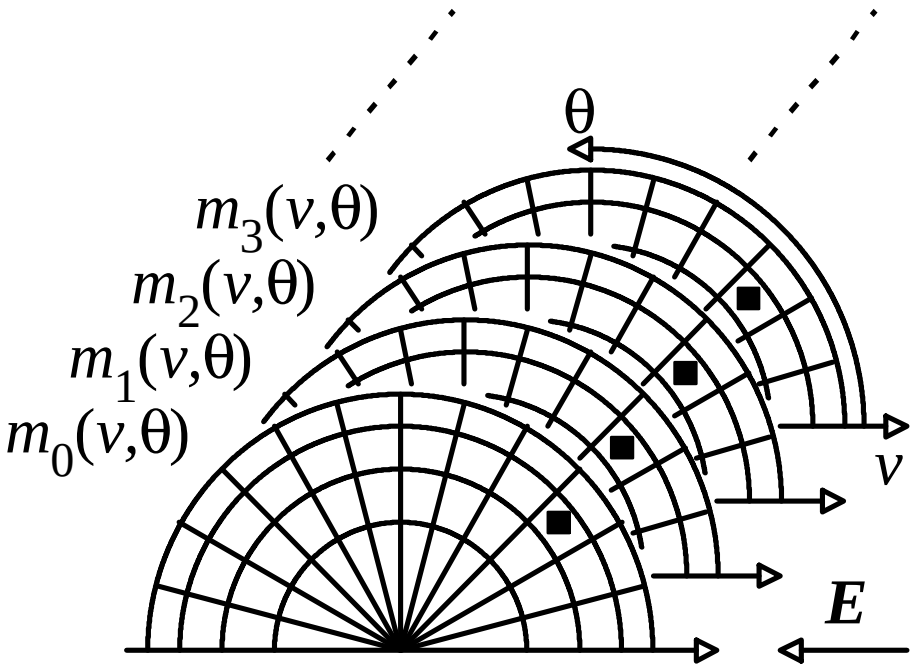

Figure 1. Cells for the calculation of the spatial moments. Two-dimensional velocity space (v; í) is divided into cells. The cells with full squares, for example, are at the same velocity. Each cell has the amount of the corresponding order of moment of the electrons in the cell $m_n(v; í)dvd í$.

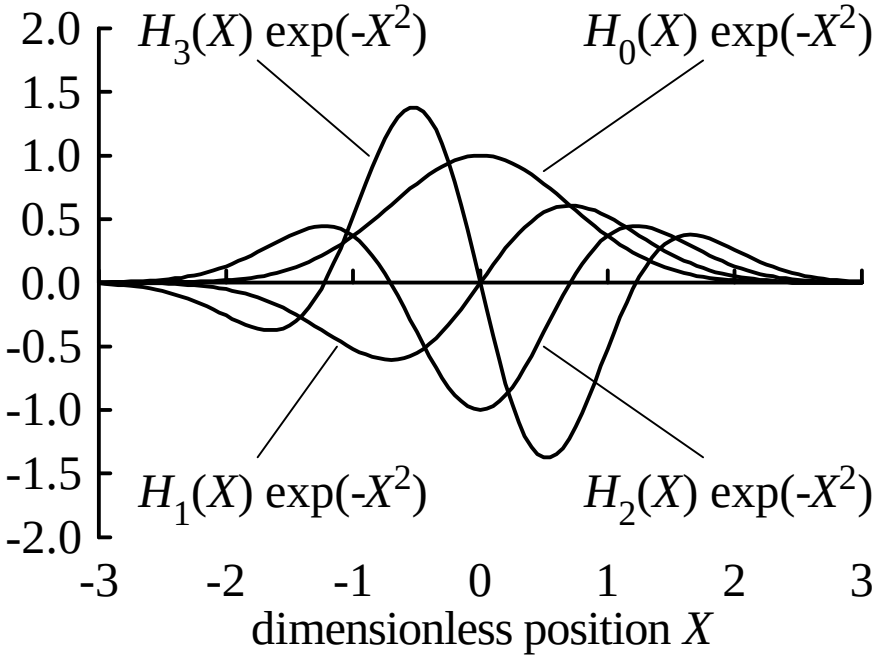

Figure 2. Forms of Hermite components $H_n(X)\exp(\ddot{A}X^2)$ (n = 0; 1; 2; 3).

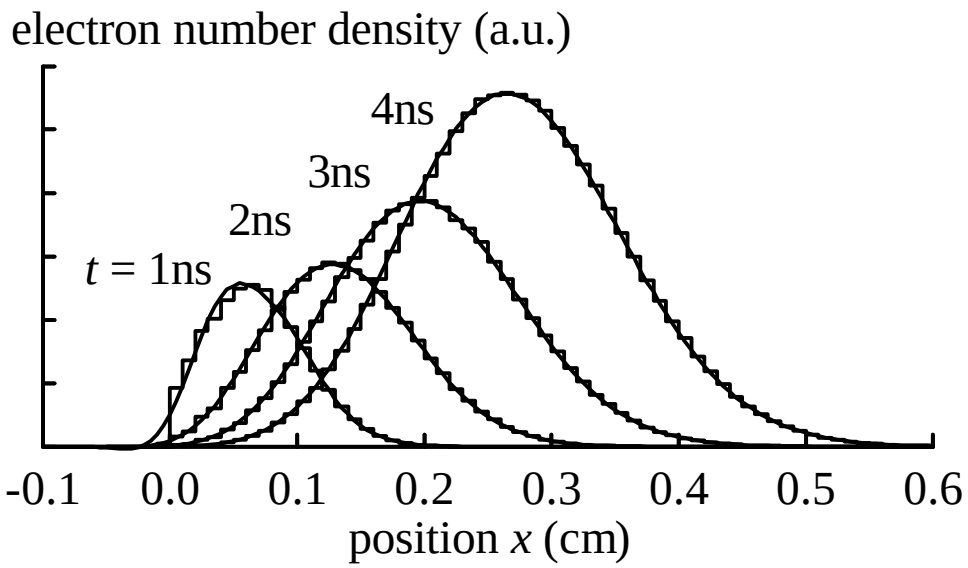

Figure 3. The spatio-temporal development of an electron swarm in SF_6 at E = 500 V cmÄ1 and p = 1 Torr (E=N = 1414 Td): histogram, Monte Carlo simulation (MC); and full curve, propagator method (PM). In the MC, electrons are directly sampled at each position. In contrast, the PM calculates the simultaneous moment equations in velocity space, then the spatial distribution is constructed using a Hermite expansion technique based on the calculation results of the spatial moment.

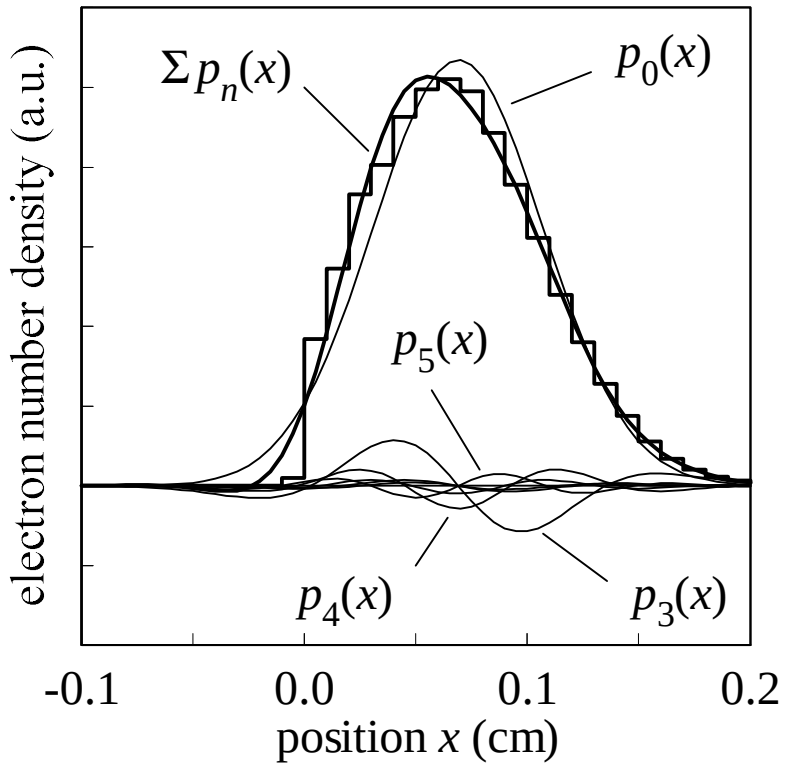

Figure 4. The composition of the spatial distribution of electrons in SF_6 at t = 1 ns using Hermite components $p_n(x)$ calculated by the propagator method. The histogram is the result of a Monte Carlo simulation.

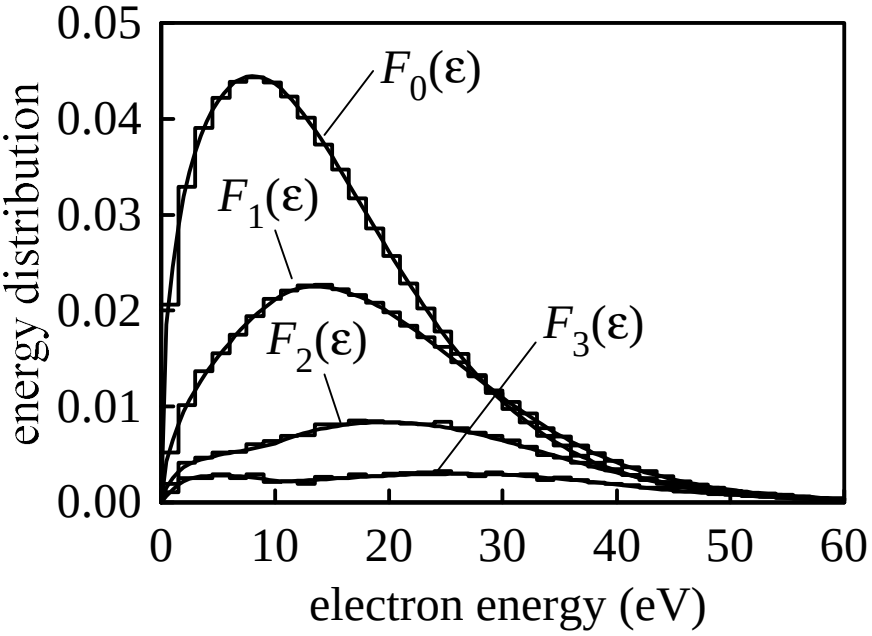

Figure 5. The electron energy distribution in SF_6 at E=N = 1414 Td: histogram, Monte Carlo simulation; and full curve, propagator method. $F_n(\varepsilon)$ is the nth-order term of the Legendre expansion calculated from $m_0(v; \iota)$.

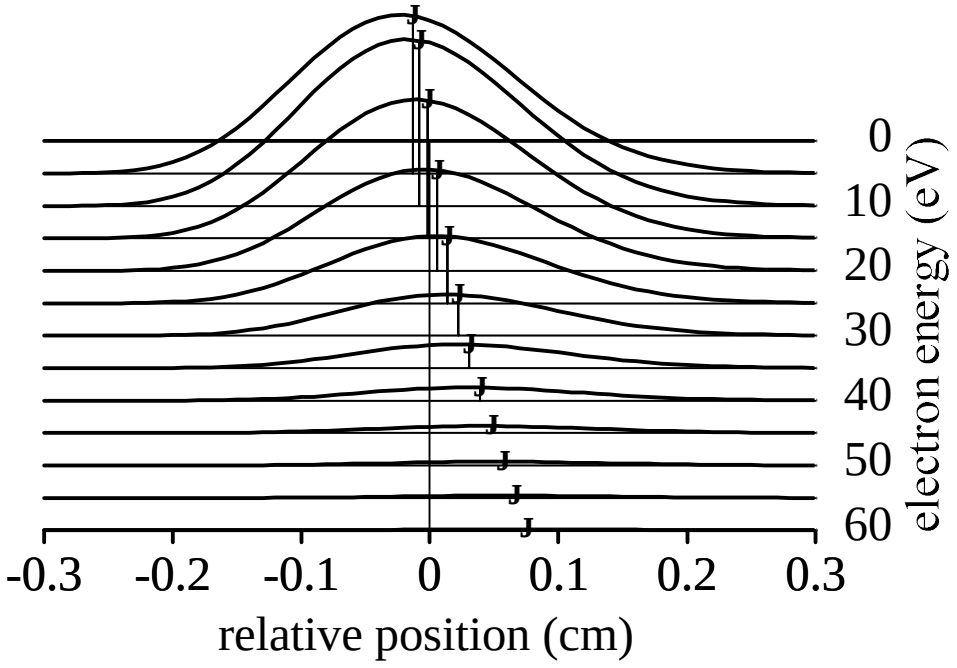

Figure 6. The energy-resolved spatial electron distribution $p(x; \varepsilon)$ in SF_6 at E=N = 1414 Td and t = 4 ns calculated by a propagator method. $p(x; \varepsilon)$ is represented as a function relative to the centroid of the entire electron swarm. Each full circle represents the centroid position of $p(x; \varepsilon)$ at the corresponding electron energy ε. High-energy electrons are shifted forward within the electron swarm; however, the electrons with energies higher than ε_{ion} = 15:8 eV are distributed almost throughout the entire range of the swarm, keeping their forms close to Gaussian distributions.

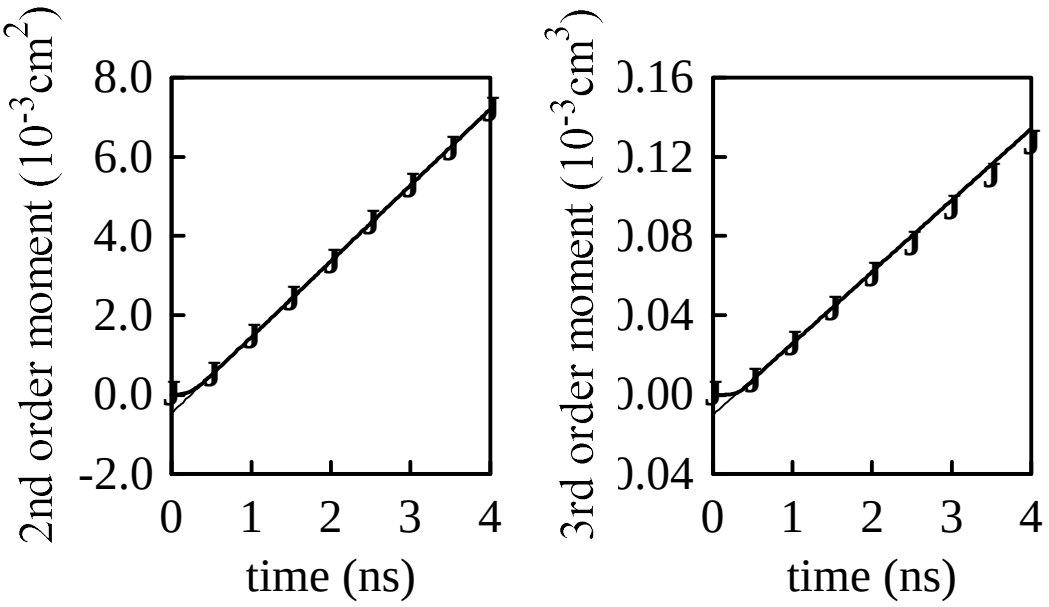

Figure 7. Relaxation of the moments m_n: full circles, Monte Carlo simulation; and full curves, propagator method. The central moment m_n is equivallent to the cumulant $\hat{\imath}_n$ for n = 2 and 3. The diãusion coeécients are obtained as $D_L = (dm_2=dt)=2!$ and $D_3 = (dm_3=dt)=3!$. The inçuence of the relaxation process of the electron swarm appears as $m_{2;0}$ and $m_{3;0}$ which are obtained from the points of interaction between the åtting lines and the vertical axes. The inçuence of $m_{2;0}$ and $m_{3;0}$ is eãectively small in long-time solution.

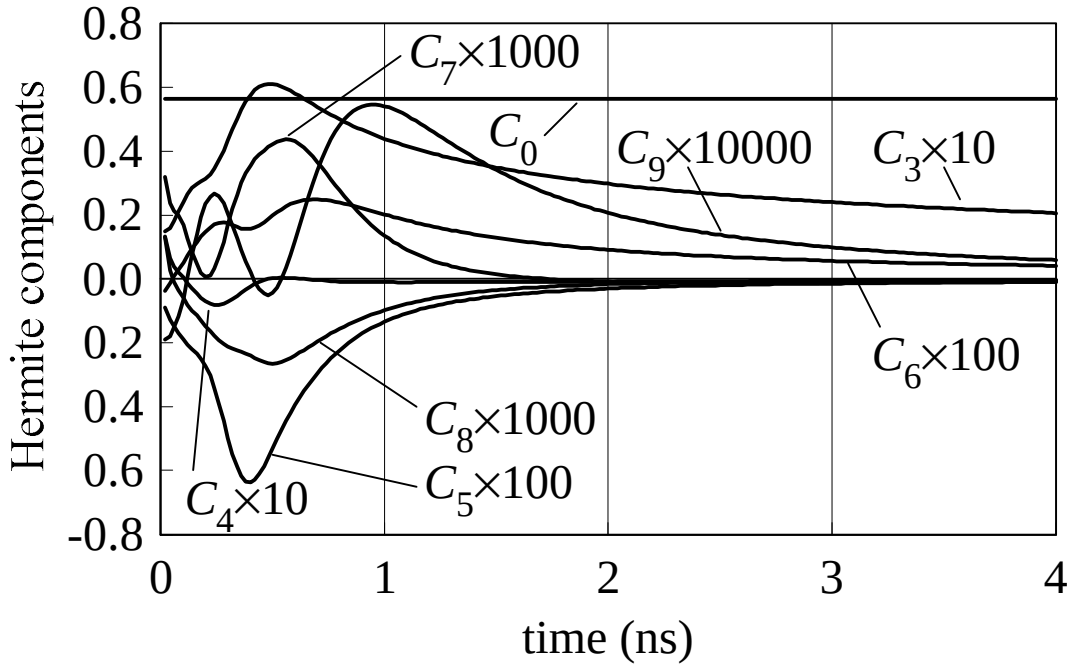

Figure 8. The temporal decays of the weights of Hermite components $C_n=m_0$ of the spatial electron distribution p(x) in SF_6 at E = 500 V $cm^{Ä1}$ and 1 Torr (E=N = 1414 Td). It is assumed that p(x) is given as a normalized function relative to the centroid of an electron swarm; thus, m_0 = 1, C_0 = $ô^{Ä1=2}$ and C_1 = C_2 = 0. The decays of C_3, C_6 and C_9 are slow due to an eãect of the third order diãusion coeécient D_3.