Letter

# Space-resolved average kinetic energy of ion swarms in a uniform electric field

Z. M. Raspopović
*Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia*

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A pulse of noninteracting charged particles in an unbounded gas, exposed to a low, constant, homogeneous electric field, was studied in both space and time using a Monte Carlo simulation technique. The difference in electrical potential between the leading and trailing edges of the swarm results in the space-resolved average ion kinetic energy becoming a linearly increasing function of space. This Letter analyzes whether the average ion kinetic energy at the leading edge reaches a stationary value during the spatiotemporal evolution of the swarm, as has been considered so far. When the swarm's mean kinetic energy reaches a steady-state value, indicating that an energy balance is established over time, the gains (from the field) and losses (due to collisions) are nonuniform across space. The local power balance is negative at the front of the swarm and positive at the tail. Cooling the ions at the front and heating the ions at the tail results in a decrease in the average ion kinetic energy at the front and an increase at the tail. Thus, it can be concluded that stationary values of average ion kinetic energy do not exist at the leading and trailing edges during the evolution. Instead, they tend to approach the swarm's mean kinetic energy as $t \to \infty$.

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*Introduction*. Today, many technologies use directional ions as one of the basic tools for etching [1] in microdischarges [2], nanotechnologies [3], and biomedical applications [4]. Tremendous resources are being invested in the advancement and development of these technologies to increase their accuracy [5]. Knowledge of the space-resolved density and average energy of charged particles during swarm evolution is in many cases crucial for understanding a great variety of basic mechanisms of physical and chemical processes between charged particles and background gas.

So far, transient and steady-state spatial profiles of the transport properties of electron swarms were investigated using a Monte Carlo simulation technique by Suvakov *et al.* [6], Raspopovic *et al.* [7], and Dujko *et al.* [8].

The physics of charged-particle swarms has always formed the foundation for the modeling of nonequilibrium plasmas. Swarm experiments and the associated transport theory of swarm particles are often used to determine the cross sections and/or interaction potentials. On the other hand, fluid models of plasma discharges require swarm transport coefficients as a function of the applied electric field.

In the work [8], it was found that full spatial relaxation is achieved under conditions when diffusion fluxes due to gradients in electron number density are much smaller than the corresponding drift due to the electric field force. Only under these conditions is the swarm fully relaxed in space, and local velocities at the leading and trailing edges of the swarm remain unchanged in time.

In the context of swarm studies, the spatial variation of the average ion kinetic energy along the swarm has played a central role in the explanation of many phenomena, including those associated with the implicit and explicit effects of nonconservative collisions and the anisotropic nature of the diffusion [9–11]. The duality of the transport coefficients, e.g., the existence of two families of transport coefficients, the flux and the bulk [12], is explained in terms of the anisotropic distribution of the average ion kinetic energy along the swarm and energy dependent collision frequencies for nonconservative collisions. The present Letter contributes to this body of research by calculating the evolution of the average kinetic energy along the swarm and exploring its properties.

The present study aims to (i) present the relaxation of the spatial profiles of transport properties of ions in the uniform electric field, and to determine their steady-state profiles. Special attention is paid to (ii) determining whether the average ion kinetic energy at the leading edge reaches some constant stationary value or decreases during swarm evolution and (iii) identifying the spatial locations where drifting ions gain and where they lose energy during swarm evolution.

This Letter is organized as follows: First, the model used is presented, and then a brief description of the Monte Carlo technique for simulating the spatiotemporal swarm evolution is given. Results and discussion, the initial conditions of the simulation are provided next. Along with a description of the temporal relaxation. Then the relaxation of the space-resolved properties along the field direction, including ion number density and average ion kinetic energy, are presented. Energy gains and losses of the drifting ions are then presented. Finally, the results are discussed and compared with the findings of prior studies, and based on that, the conclusion is reached. Additionally, Supplemental Material is provided to accompany the Letter.

*Model approach*. A swarm, i.e., a dilute gas of charged particles that collide with background gas particles at a temperature, $T$, moves under the influence of an external electric field ($\boldsymbol{E}$) in an infinite space ($x, y, z$). The ensemble of ions has sufficiently low density so that (i) mutual interactions between ions can be neglected; (ii) the background neutral gas remains essentially undisturbed, and (iii) space-charge fields are negligible in comparison with the applied field.

 

The duration of collisions is negligible compared to the mean time between two collisions. This means that all quantum-mechanical phenomena are exclusively described by collision cross sections, and the motion of a swarm of charged particles can be described by the laws of classical physics. Using the language of plasma physics, this physical system is usually referred to as the swarm of charged particles, or sometimes the so-called test particle limit.

A swarm of lithium ions ($^7Li^+$) in krypton gas ($^{88}Kr$) was studied. This is simply an artificial condition of basic research. We assume that the interaction between ions and atoms takes place under the influence of an induced dipole force, which corresponds to the momentum transfer cross section for elastic collisions:

$$\sigma_{\mathrm{MT}}(\dot{\mathrm{A}}^2) = 29/\sqrt{E(\mathrm{eV})}.$$

The $\sigma_{\mathrm{MT}}$ includes anisotropic backward and forward scatterings, as well as the isotropic capture part.

Although the model describing the interaction of ions and background gas particles has a constant collision frequency of 55.6 MHz, i.e., the mean collision time of $t_c = 1.8 \times 10^{-8}$ s, which means that it is very simple, in this case, it is also completely realistic. In the range of reduced electric field strength $|\boldsymbol{E}|/N_g < 25$ Td (1 Td $= 10^{-21}$ V m$^2$, $N_g$ is the gas number density), computed drift velocities by Koutselos *et al.* [13], Lozeille *et al.* [14], and Tan *et al.* [15], as well as in the presented simulations, agree well (<1%) with those experimentally measured by Ellis *et al.* [16] and Takebe *et al.* [17] at $T = 300$ K.

*Monte Carlo simulation*. The code used in these simulations was verified on benchmark tests [18]. It is based on tracking a large number of ions that gain the energy from the external electric field directed along the $z$ axis and dissipate this energy through collisional transfer with neutral gas particles. Collisions are instantaneous and isotropic, and the instant of collision is determined by the null-collision method [19].

Swarm transport parameters (averaged on all of the swarm, such as the mean kinetic energy and drift velocity) and the space-resolved transport properties of ions (such as the average kinetic energy and number density) were observed through the temporal evolution for the sampling instants. When the swarm's mean energy $E(t_s)$ and drift velocity $v_d(t_s)$ reach their steady-state values they are denoted by $E_s$ and $v_d$.

For sampling of the one-dimensional space-resolved transport properties of ions along the electric field direction, the space of the swarm is restricted in interval $z \in (z_{\mathrm{c.m.}} - 3\sigma_z,\ z_{\mathrm{c.m.}} + 3\sigma_z)$, where $z_{\mathrm{c.m.}}$ is the coordinate of the centers of mass (c.m.) of the swarm, and $\sigma_z = (\langle z^2\rangle - \langle z\rangle^2)^{0.5}$ is the standard deviation of the spatial distribution of ions along the electric field. The mean value of magnitude $A$ is denoted as $\langle A\rangle$. The observed spatial interval is divided into $N_b$ cells whose centers have $z_p$ coordinates and these points are used to sample spatial profiles of the swarm. This study follows the development of the swarm in real space as well as in space normalized to six standard deviations ($6\sigma_z$). The width of the cell in real space increases with time as $\Delta z(t) = 6\sigma_z(t)/N_b \propto t^{0.5}$, while in normalized space it does not increase $\Delta\sigma(t) = 6/N_b =$ const.

In this Letter, we present the computation of one-dimensional spatial profiles of the transport properties of the ions along the direction of the field. These properties of the ions include the number density of the ions, $N(z,\ t)$; the average ion kinetic energy, $E(z,t)$; the average ion velocity, $v_z(z,t)$; the average electric power absorbed from the electric field by the ions, $P_E(z,t)$; and the average ion dissipated power losses due to collision processes, $P_C(z,t)$. The space-resolved number density of the ions, $N(z_p,t_s)$, represents the number of ions in the spatial cell $p$ for the instants $t_s$ per the width of the spatial cell, normalized to the total number of the ions, which is the same as the distribution function of the swarm along the $z$ axis.

*Results and discussion*. In this section, the spatiotemporal evolution of drifting lithium ions in the background gas of krypton at a temperature of $T = 300$ K was considered in a reduced electric field strength of $|\boldsymbol{E}|/N_g = 20$ Td, where the gas number density was set to $3.54 \times 10^{22}\,\mathrm{m}^{-3}$. At time $t = 0$, corresponding to a delta-function pulse in time, the ions are initially isotropically released from the origin according to the Maxwellian distribution, with a mean starting energy of $E_0 = 0.1$ eV. After approximately 50 collisions per ion or about 1 μs, the total balance of momentum and energy is established, i.e., drift velocity and swarm main kinetic energy have reached their steady-state values of $v_d = 188$ m/s and $E_s = 0.0555$ eV.

*Spatiotemporal relaxation of the ion number density and average ion kinetic energy*. At the beginning of the initial collision-free phase until the moment $t = 0.1$ ns, there were practically no collisions between the ions and the gas particles ($t/t_c = 0.0056$). In such a short time, the electric field has negligibly changed the individual ion energies in relation to their initial values at the origin. As a consequence, the ions generally occupy simple positions corresponding to their starting energy. For times sufficiently short after the instant of isotropic emission, the swarm will display spherical symmetry in three-dimensional space, with ions of the same initial energy assuming positions on a sphere whose radius is dependent on their energy [$r = (2E/m)^{0.5}t$].

The one-dimensional spatial profile of the $N(z)$ has a Gaussian shape while the profile of the $E(z)$ has the shape of a parabola (Fig. 1). Figure 1 shows that the $E(z)$ around the c.m. is less than the mean starting energy $E_0$. The c.m. neighborhood for that instant contains only ions that have a small velocity component along or opposite to the field, in order for ions to remain in the central spatial cell ($z < 0.5\Delta z$).

When the swarm accelerates, the maximum of the $N(\sigma)$ profile moves backwards relative to the c.m., shown in Fig. 2. Afterwards, when the total balance of momentum is established, the collisions shift the maximum back towards the c.m. Figure 2 also shows the Gaussian function (gray symbols), which represents the shape to which the profile of the $N(\sigma)$ approaches during its further evolution.

Figure 3 displays the $N(z)$ profiles as solid lines and the $E(z)$ profiles as symbols, for the instants of 0.5, 1, 1.5, and 2 μs. The swarm has not yet completely passed the origin (situated at $z = 0$), and the swarm transport parameters have already reached their steady-state values ($t > 1$ μs).

Between $t = 0.1$ ns and 2 μs there is a significant evolution of the $E(z)$, as shown in Figs. 1 and 3. It changes from a

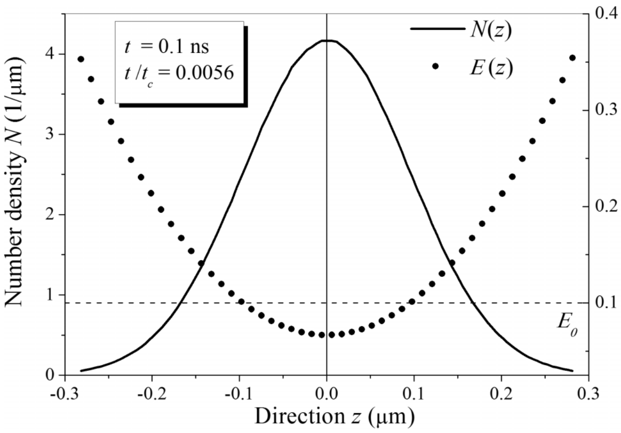


FIG. 1. Space-resolved ion number density and average ion kinetic energy, for the instant of $t = 0.1$ ns.

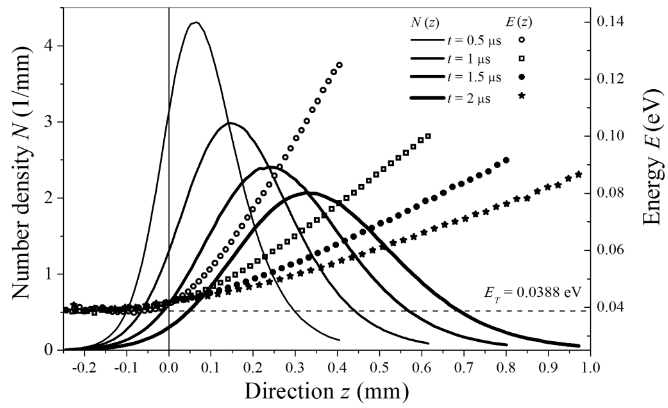


FIG. 3. Space-resolved ion number density (solid lines) and average ion kinetic energy (symbols), for the instants when the swarm did not leave the origin yet. $E_T$ represents the thermal energy of the background gas.

symmetric distribution to an asymmetric distribution with a much lower $E(z)$, and with the ions behind the c.m. having energy close to the thermal energy of the gas. The evolution of the shape of the $E(z)$ profile, from a parabolic to a linearly increasing function of space, is due solely to the field and the initial conditions. However, collisions can erase the local memory of the initial conditions.

Figure 4 shows that for the instant of $t = 100$ μs the profile of the $N(\sigma)$ coincided with the Gaussian shape. This coincidence does not mean that the $N(\sigma)$ is spatially relaxed, but only that the displacement of the maximum of the $N(\sigma)$ profile relative to the c.m. is less than half the width of the spatial cell $(0.5\Delta\sigma)$ for that instant.

After some point in the swarm evolution, the simulations used cannot determine the behavior of the slope of the $E(\sigma)$ line due to its small changes with time as shown in Fig. 4.

Although the slope of the steady-state profile of the $E(\sigma)$ cannot be determined by these simulations based on profile slope monitoring, it can be sought based on the spatial locations where the ions gain and lose energy during swarm relaxation.

*Spatiotemporal relaxation of the energy gains and losses of the drifting ions*. The nature of the spatial profile of the transport properties of ions is dependent on the interplay between the local electric and dissipated power. The work done by an ion while moving in a constant uniform electric field is proportional to the displacement of ions along the direction of the field. In the absence of nonconservative collisions [12], the local average electric energy absorbed by ions from the field is proportional to the local average ion velocity $[\Delta E(z) \propto v_z(z)\Delta t]$. The energy transmitted between an ion and a gas particle during an elastic collision is proportional to the ion kinetic energy. The local average dissipated energy by ions due to collision processes is proportional to the local average ion kinetic energy $[\Delta E(z) \propto E(z)\Delta t/t_c]$. Due to the different functional forms when total energy balance is established, local electric gains and dissipated losses of energy are generally not in balance. In this section, the spatiotemporal relaxation of the electric and dissipated power spatial profiles, and the associated phenomena induced by nonlocal effects are shown.

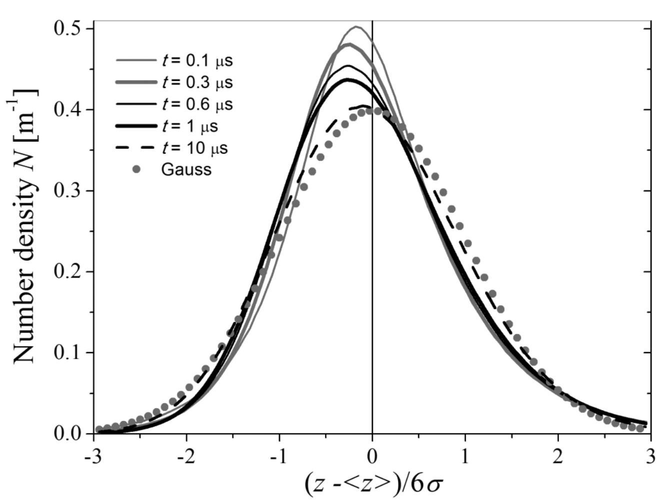


FIG. 2. Space-resolved ion number density in the normalized space for different instants.

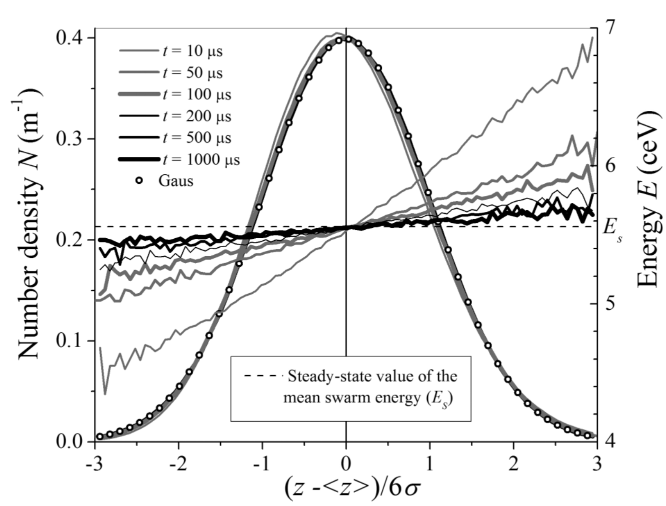


FIG. 4. Space-resolved ion number density (like Gaussian shape) and average ion kinetic energy (linearly increasing functions of space) for different instants in which they aspire to their steady-state forms.

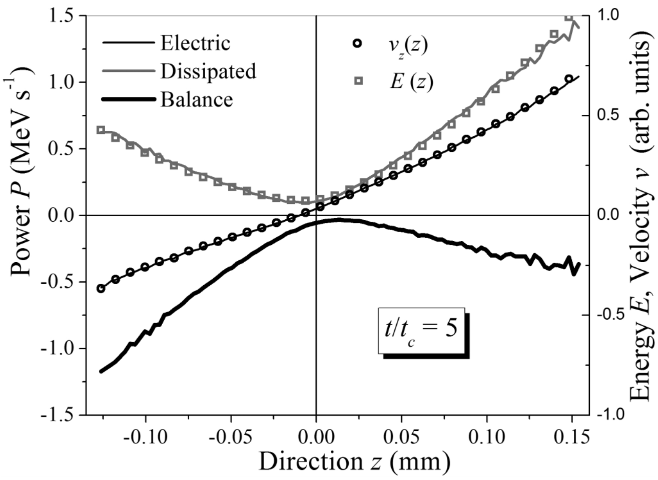


FIG. 5. Space-resolved average ion power including average ion electric power, average ion dissipative power losses, and average ion power balance for the instant of $t = 5t_c$. The units for $E(z)$ and $v_z(z)$ profiles were chosen for the curves to overlap the power profiles.

During the relaxation of the swarm's mean kinetic energy from its starting value of 0.1 eV to its steady-state value of 0.056 eV, for the instant of $t/t_c = 5$, the local average power balance, $P(z)$, is less than zero in the whole swarm space, as we can see in Fig. 5. The spatial profile of the average dissipated power due to collision processes, $P_C(z)$, for that instant, coincided with the shape of the $E(z)$ profile, while the profile of the average power deposited into ions by the electric field, $P_E(z)$, coincided with the shape of the $v_z(z)$ profile, according to their functional dependencies. The $E(z)$ and $v_z(z)$ profiles are shown as symbols in Fig. 5.

During the further swarm evolution, the $P_E(z)$ and $P_C(z)$ profiles are linearly increasing functions of space as shown in Fig. 6. The fact that the slope of the $P_C(z)$ profile is higher than that of the $P_E(z)$ profile, leads to a conclusion that $P(z) < 0$ at the swarm front, while $P(z) > 0$ is at the tail.

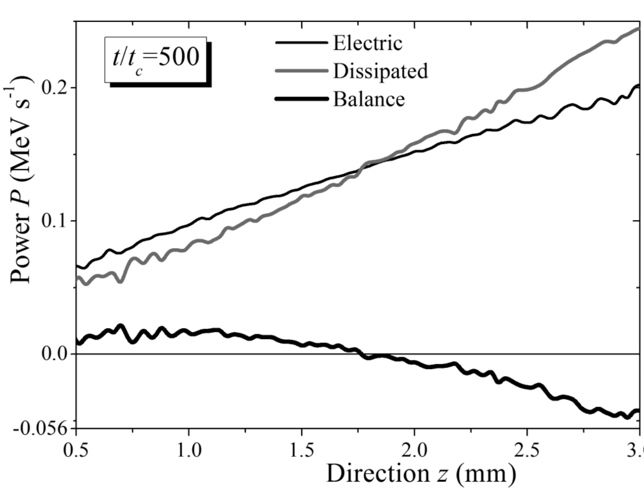


FIG. 6. Space-resolved average ion power including average ion electric power, average ion dissipative power losses, and average power balance of the ions for the instant of $t = 500t_c$.

In real space, the slopes of the $E(z)$, $v_z(z)$, and $P(z)$ profiles decrease due to both the increase in swarm dimensions caused by diffusion and the shape of the $P(z)$ profile. However, in normalized space, their decrease is due to the shape of the $P(\sigma)$ profile. Furthermore, the behavior of local ion kinetic energies at the leading and tail edges of the swarm is more clearly observed in normalized space, as shown in Fig. 4. Cooling the front and heating the tail of the swarm results in a decrease in the slope of the $E(\sigma)$ and $v_z(\sigma)$ profiles, and less difference between $P_E(\sigma)$ and $P_C(\sigma)$. This self-consistent decrease in the slope of the $E(\sigma)$ and $v_z(\sigma)$ profiles on the one hand, and the decrease in the slope of the $P(\sigma)$ profile on the other, causes a slower change in the slope of the $E(\sigma)$, $v_z(\sigma)$, and $P(\sigma)$ profiles over time. When $t \to \infty$, the energy gain and loss mechanism becomes locally balanced and spatially independent, causing the $P(\sigma)$ profile to approach its steady-state form of zero slope and constant zero value.

The Supplemental Material [20] contains a comparison of the $P(z)$ and $P(x)$ profiles. Here, the $x$ direction denotes any direction perpendicular to the field. The $P_C(x)$ profile follows the shape of the $E(x)$ profile, which, due to free diffusion, resembles spreading parabolas. In contrast, the $P_E(x)$ profiles are constant, independent of $x$. Different forms of the $P_C(x)$ and $P_E(x)$ result in $P(x) > 0$ near the c.m., and $P(x) < 0$ at the periphery of the swarm.

*Conclusion*. During the final phase of relaxation of a swarm of charged particles in a constant electric field, the interplay of electrical gains and losses in the elastic collisions of ions, leads to the shape of the $P(z)$ profile as a linearly decreasing function of space, with zero in the c.m. and with a slope approaching zero.

The $E(z)$ changes from the initial parabolic shape, due to the initial condition, to a linearly increasing function of space, due to the electric field. In the final phase of relaxation the local value of the $E(z)$ on the leading edge decreases, while on the trailing edge, it increases. This is a result of the shape of the $P(z)$ profile. When $t \to \infty$, the $E(z)$ profile tends to its steady-state shape, and becomes spatially independent and locally equal to the mean energy of the swarm, despite the significant difference in electrical potential between the leading and trailing edges of the swarm. This is not in accordance with the conclusion of the work [8], given in the Introduction.

The obtained steady-state spatial profiles of the transport properties of ions for very simple so-called "closed-shell" systems, such as $^7Li^+$ in $^{88}Kr$, can also be generalized to systems, in which there are different ion-neutral interactions. These are primarily systems in which (1) the total collision frequency increases with energy or (2) the ion energy losses in the collision increase in relation to the losses in elastic collisions. Examples for the first group are the soft sphere scattering models, for which $\nu(E) \propto E^n$ is satisfied, where $n \in (0, \frac{1}{2})$, as well as the hard spheres scattering model [$\sigma_{\mathrm{MT}} = \mathrm{const} \to \nu(E) \propto E^{1/2}$]. The second group includes systems, in which inelastic collisions, neutral dissociation, ionization, or symmetric charge-exchange collisions exist between charged particles and background gas.

The presence of the mentioned ion-neutral interactions (1) and (2) in the plasma results in a greater energy exchange between ions and gas at higher ion kinetic energies compared to the considered elastic interaction. As a result, these interactions accelerate the relaxation process of the swarm and facilitate the formation of ion spatial profiles that correspond to those depicted in this study.

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[20] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevE.108.L053202 for longitudinal and perpendicular spatially resolved profiles of average powers during the swarm evolution.