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Space charge effects in ultrafast electron diffraction and imaging

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In a recent article [J. Appl. Phys. 92, 1643 (2002)] Siwick et al. investigated the space-charge-limited electron pulse propagation in a photoelectron gun using an analytical approach, referred to as mean-field theory, and a numerical N-body simulation. The results were compared with a one-dimensional fluid model [J. Appl. Phys. 91, 462 (2002)], and a conclusion was made that the fluid model overestimates the pulse duration after a certain propagation time. Although the mean-field theory and N-body simulation give exactly the same results for all examples studied, we point out that the expression for the on-axis potential in their mean-field model is inapplicable to investigating the electron space-charge dynamics in an ultrafast electron packet. We correct that expression and derive a two-dimensional model that is in agreement with our previous one-dimensional fluid model. We also point out several areas where Siwick et al. have misinterpreted the one-dimensional fluid model.

Recently, Siwick et al. published an article on the propagation dynamics of femtosecond electron packets in the drift region of a photoelectron gun using an analytical model they referred to as a mean-field (MF) model, and a numerical N-body simulation. The predictions of their model were compared to a one-dimensional (1D) fluid model described in Ref. 2, and they concluded that the fluid model overestimates pulse broadening after a certain drift time. We find that the MF theory of Ref. 1 is based on an assumed on-axis potential that incorrectly models the space-charge-limited electron dynamics in an ultrafast photoelectron gun. We solve for the correct potential and develop a two-dimensional (2D) model that shows agreement with our previous 1D fluid model. We also point out areas which the authors of Ref. 1 misinterpreted the model in Ref. 2.

In Ref. 1, the expression

\[ V(z) = \frac{Ne}{2\varepsilon_0 \pi r_b^2} \left[ \sqrt{z^2 + r_b^2} - z \right] \]  

(1)

was used to describe the on-axis potential distribution of an electron disk with radius \( r_b \) and length \( l \) as shown in Fig. 1. The center of the electron disk is at \( z = 0 \). In Eq. (1), \( N \) is the total number of electrons contained in the electron pulse (EP), \( -e \) is the electron charge, and \( \varepsilon_0 \) is the vacuum permittivity.

The authors of Ref. 1 indicated that they obtained Eq. (1) from Ref. 3, in which it was derived assuming that the electron disk is infinitely thin (\( l = 0 \)), a condition that is inapplicable for describing an EP with a finite length of \( l \neq 0 \). Thus, Eq. (1) cannot be used for investigating the space-charge effects inside the EP. In addition, the central equation of their model,

\[ \frac{d^2l}{dt^2} = \frac{Ne^2}{m\varepsilon_0 \pi r_b^2} \left( 1 - \frac{l}{\sqrt{l^2 + 4r_b^2}} \right) \]  

(2)

is also incorrect because it is derived from Eq. (1) based on \( l = 0 \).

One can easily obtain from Eq. (1) the on-axis electric field, which is expressed as

\[ E_z = -\frac{\partial V}{\partial z} = \frac{Ne}{2\varepsilon_0 \pi r_b^2} \left[ \frac{z}{\sqrt{z^2 + r_b^2}} - 1 \right] \]  

(3)

Thus, one can see that the electric field \( E_z = -Ne/(2\varepsilon_0 \pi r_b^2) \neq 0 \) at \( z = 0 \). This is physically incorrect for an EP propagating in free space. The electron at the center of the symmetric electron disk, \( z = 0 \), should feel no force, and therefore \( E_z = 0 \) at \( z = 0 \).

A correct potential would account for the finite length \( l \) of the electron packet. The Poisson equation for the problem of Fig. 1 can be written as

\[ \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial \phi}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 \phi}{\partial \theta^2} + \frac{\partial^2 \phi}{\partial z^2} = \frac{en(r, \theta, z)}{\varepsilon_0} \]  

(4)

where \( \phi = \phi(r, \theta, z) \) is the potential distribution in free space and \( n = n(r, \theta, z) \) is the electron density. In order to solve Eq. (4), one can use the Green’s function.
The electron density is assumed to be spatially constant, and therefore the potential distribution is in the form of \( V(r, r', \theta, \theta', z, z') \)

\[
G(r, r', \theta, \theta', z, z') = \frac{1}{\sqrt{r^2 + r'^2 - 2rr' \cos(\theta - \theta') + (z - z')^2}}, \tag{5}
\]

satisfying

\[
\frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial G}{\partial r} \right) + \frac{\partial^2 G}{\partial z^2} = -\frac{4\pi}{m} \delta(r - r') \delta(\theta - \theta') \delta(z - z'), \tag{6}
\]

to give the solution of \( \phi = \phi(r, \theta, z) \), which is expressed as

\[
\phi = -\frac{e}{4\pi\epsilon_0} \int_{\nu'} n(r', \theta', z') G(r, r', \theta, \theta', z, z') r' dr' d\theta' dz'.
\]

The electron density is assumed to be spatially constant, and therefore the potential distribution is in the form of \( V(z) = \phi(0, z) \), and can be expressed as

\[
V(z) = -\frac{Ne}{2\epsilon_0 m r_b^2} \left\{ \frac{1}{2} \left[ \frac{1}{2} - z \right] + \sqrt{\left[ \frac{1}{2} - z \right]^2 + r_b^2} \right. \\
\quad + \frac{1}{2} \left[ \frac{1}{2} + z \right] \sqrt{\left[ \frac{1}{2} + z \right]^2 + r_b^2} \\
\quad + \frac{r_b^2}{2} \ln \left[ \frac{1}{2} - z + \sqrt{\left[ \frac{1}{2} - z \right]^2 + r_b^2} \right] \\
\quad - \frac{r_b^2}{2} \ln \left[ -\frac{1}{2} - z + \sqrt{\left[ \frac{1}{2} + z \right]^2 + r_b^2} \right] \\
\left. - \frac{1}{2} \left[ \frac{1}{2} - z \right] \left[ \frac{1}{2} + z \right] - \frac{1}{2} \left[ \frac{1}{2} + z \right] \left[ \frac{1}{2} + z \right] \right\}. \tag{8}
\]

In the limit of \( l = 0 \), Eq. (8) exactly reduces to Eq. (1). The longitudinal electric field can be expressed as

\[
E_z = -\frac{\partial V}{\partial z} = \frac{Ne}{2\epsilon_0 m r_b^2} \left[ \sqrt{\left[ \frac{1}{2} - z \right]^2 + r_b^2} \\
- \sqrt{\left[ \frac{1}{2} + z \right]^2 + r_b^2} + \frac{l}{2} - z - \left[ \frac{l}{2} + z \right] \right]. \tag{9}
\]

Therefore, the correct form of Eq. (2) should be

\[
\frac{d^2l}{dt^2} = -\frac{e}{m} E_z \bigg|_{z=-l/2} + \frac{e}{m} E_z \bigg|_{z=-l/2} \\
= \frac{2Ne^2}{m\epsilon_0 \pi r_b^4 \left( 1 + 2l/r_b + \sqrt{1 + l^2/r_b^2} \right)}.
\tag{10}
\]

where \( m \) is electron rest mass.

One can see that Eq. (10) is different from Eq. (2) which is the central equation of the MF theory of Ref. 1, based on the assumption of \( l = 0 \). It is noticed that the value of \( E_z \) given by Eq. (9) is \( E_z = 0 \) at \( z = 0 \), which is physically correct for the model shown in Fig. 1. Therefore, one should use Eq. (10) to investigate the space-charge-limited EP in a photoelectron gun. We do not know why the MF theory and the N-body simulation of Ref. 1 gave exactly the same predictions in all cases since the details of the N-body simulation were not given. However, Eq. (2) used in the MF model obviously represents an incorrect geometry for representing the electron packet.

In addition to the error in setting up the on-axis potential distribution, in Ref. 1, several misinterpretations of the 1D fluid model of Ref. 2 were made. The 1D fluid model investigating pulse broadening is limited to the condition that the electron-beam radius \( r_b \) is larger than its length \( l \). This condition on the applicability of 1D models is common knowledge that can be found in conventional books of plasma physics and beam physics, (for example, see Ref. 4). In the case of \( l/r_b \ll 1 \), Eq. (10) reduces to the result of the 1D fluid model.\(^2\) The purpose of Ref. 2 is to derive an analytical solution for a 1D fluid model since there is no analytical solution for Eq. (10). In Ref. 2, the investigation focuses on femtosecond photoelectron guns with beam radius \( r_b = 0.2–0.5 \) mm and pulse length of about 200–2000 fs, corresponding to \( l = 0.02–0.2 \) mm for an electron energy of 30 keV. These parameters satisfy the 1D limit, as do all parameters discussed in Ref. 2. However, the authors of Ref. 1 gave some parameters that did not satisfy the 1D limit, but had \( l/r_b \gg 1 \), and applied these parameters to the 1D model, thus violating the basic assumptions behind that analytical model.

We next compare the predictions of the present 2D model with the 1D fluid model of Ref. 2. Figure 2 shows the EP broadening \( \Delta t = l/v_b \) (where \( v_b \) is EP velocity) as a function of EP drift time \( t \) for initial EP duration of \( t = 50 \) fs, electron initial energy of 30 keV, \( r_b = 0.4 \) mm, and \( N = 1000 \), in the cases of 1D and 2D models. As can be seen from Fig. 2, the results of both 1D and 2D models almost coincide because the parameters in Fig. 2 satisfy the condition of the 1D limit \( l/r_b \ll 1 \). Due to the 1D limit, the 1D model is suitable for analyzing femtosecond photoelectron guns, but becomes inaccurate when the EP duration develops.
into the picosecond regime especially for the smaller electron-beam radius. In Ref. 1, the limitations of the 1D treatment were neglected, and thus some improper application of that model was made.

Figure 3 shows the difference between the 2D model using the correct potential described by Eq. (8) and the MF theory of Ref. 1 which used the potential described in Eq. (1). In Fig. 3, the EP broadening $\Delta t = l/v_b$ is plotted as a function of the EP drift time $t$ for initial EP duration of $\tau = 1000$ fs, electron initial energy of 30 keV, $r_b = 0.1$ mm, and $N = 5000$, in the cases of the MF theory and the 2D model. It can be seen from Fig. 3 that the MF theory overestimates the EP broadening. The difference between the 2D model and the MF theory increases with the EP drift time.

Therefore, the MF theory is not applicable when the EP duration extends into the picosecond regime.

The absolute value $\Delta E_a$ of the electron energy spread due to space-charge effects is expressed in Ref. 2 in the electron-moving frame with moving velocity of $v_b$. This treatment of $\Delta E_a$ was introduced previously in Ref. 5 for determining beam quality and describing beam emittance caused by space-charge effects. Although the frame of reference was not explicitly stated in Ref. 2, the use of the electron-moving frame of reference is clear from the expression relating the electron energy spread to the difference in the maximum and minimum potential in the electron pulse [Eq. (24) in Ref. 2]. In this electron-moving frame, $\Delta E_a$ is independent of the electron drift velocity $v_b$, and is expressed as

$$\Delta E_a = \frac{1}{2} m \Delta v_{sp}^2,$$

where $\Delta v_{sp}$ is electron velocity spread caused by the electron beam space-charge effects. In the laboratory frame, the relative value $\Delta E_r$ of electron energy spread depends on the beam drift velocity $v_b$, and can be expressed as

$$\Delta E_r = m v_b \Delta v_{sp},$$

In Ref. 1, Eq. (12) was used to describe the energy spread in the electron bunch. The relative value $\Delta E_r$ of electron energy is a mixture of electron drift energy and space-charge effects. Obviously, $|\Delta E_r|$ decreases with $v_b$, and $\Delta E_r = 0$ when $v_b = 0$. Equation (12) is not typically used to describe the beam emittance. Alternatively, Ref. 2 used Eq. (11), which does not include the effect of drift velocity and applies to the electron-moving frame, for which one can define the

FIG. 2. The EP broadening $\Delta t = l/v_b$ as a function of EP drift time $t$ for initial EP duration of $\tau = 50$ fs, electron initial energy of 30 keV, $r_b = 0.4$ mm, and $N = 1000$, in the cases of 1D and 2D models.

FIG. 3. The EP broadening $\Delta t = l/v_b$ is plotted as a function of EP drift time $t$ for initial EP duration of $\tau = 1000$ fs, electron initial energy of 30 keV, $r_b = 0.1$ mm, and $N = 5000$, in the cases of the MF theory and the 2D model.

FIG. 4. The relative value $\Delta E_r$ of electron energy spread as a function of the EP drift time $t$ for initial EP duration of $\tau = 1000$ fs, electron initial energy of 30 keV, $r_b = 0.1$ mm, and $N = 5000$, in the cases of the MF theory and the 2D model.

FIG. 5. The absolute value $\Delta E_a$ of electron energy spread due to space-charge effects as a function of the EP drift time $t$ for initial EP duration of $\tau = 100$ fs, electron initial energy of 30 keV, $r_b = 0.4$ mm, and $N = 3000$, in the cases of 1D and 2D models.
beam emittance. Equations (11) and (12) are different definitions describing the electron energy spread.

The authors of Ref. 1 also underestimate the relative value $\Delta E_r$ of electron energy spread given by Eq. (12). This can be seen in Fig. 4, where we have plotted $\Delta E_r$ as a function of the EP drift time $t$ for initial EP duration of $\tau = 1000$ fs, electron initial energy of 30 keV, $r_b = 0.1$ mm, and $N = 5000$, in the cases of the MF theory and the 2D model. The prediction by the MF theory leads to an error of about 40% after 4 ns of propagation time, which is due to an incorrect assumption in Eq. (1). However, using the parameters satisfying the 1D limit, one can calculate the absolute value $\Delta E_a$ of the electron energy spread due to the space-charge effects, to find only a small difference between the 1D and 2D models developed by the authors of the present article. This is shown in Fig. 5, where we have plotted $\Delta E_a$ as a function of the EP drift time $t$ for initial EP duration of $\tau = 100$ fs, electron initial energy of 30 keV, $r_b = 0.4$ mm, and $N = 3000$, in the cases of 1D and 2D models. The parameters in Fig. 5 meet the requirement for the 1D limit. As can be seen from Fig. 5, the maximum difference between the two curves given by 1D and 2D models is only about 10%, which implies the 1D model is applicable in this case.

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