Alternative approach to the numerical synthesis of the dense-ion-beam focusing systems

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An alternative approach has been developed to the numerical synthesis of ion-beam focusing systems that prepare the dense laminar ion beams with the required profile of the ion trajectories. Conventionally an ill-posed synthesis problem arises in such cases, and only low-density beams with no magnetic field are treated. Instead, we compute both the electric and magnetic fields by considering two well-posed problems, the first for the equivalent potential Q and the second for the electric potential U. An analytical solution for Q for the specific case of an axial system has been found and a self-consistent method of satisfying the axial boundary conditions for Poisson's equation in U is described. It is shown that the beam can be focused while preserving its laminar structure and the required profile when applying various superpositions of both the electric and magnetic fields.

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I. INTRODUCTION

Ion and electron beams of high density are in use in many fields of modern science and technology [1–4]. The dense electron beams are required for powerful microwave and millimeter wave generators [1]. Well-formed high-power ion beams are needed for etching and modification of metal, semiconductor, and insulator surfaces [2]. Another important application is the ion doping of semiconductors when ion beams of various energy, density, and chemical composition are used to obtain the doping profiles with the required spatial configuration [3,4].

Formation of ion beams of high density is a complicated problem because of the very strong Coulomb interaction of the ions within the beam [5]. So, a magnetic field is normally required, in addition to a properly configured electric field, in order to compress a stream of accelerated ions into the dense beam of a special shape [6,7]. Unfortunately, the magnetic field essentially complicates the internal structure of the beam due to heavy mixing of the ion trajectories and the creation of a turbulent flux of particles instead of a laminar stream. This may be unacceptable for many applications when especially high precision and spatial resolution are required [4].

An intriguing question of practical importance arises in such cases as to whether it is possible to focus a dense ion beam while preserving its perfect laminar structure when both the electric and magnetic fields have been applied simultaneously. Because of the magnetic field mixing the trajectories, there is a presumption that this is generally impossible except for the trivial case of a cylindrical beam in a uniform magnetic field (the Brillouin solution) [6,7].

Apart from this question, it is a complicated problem by itself to calculate both the electric and magnetic fields in any combined electromagnetic system producing high-density ion beams [5–7]. The complications appear due to the fact that the synthesis of the focusing system is an inverse mathematical problem that is typically formulated as an ill-posed Cauchy problem for Laplace's or Poisson's equation [6]. Such a formulation is, however, inappropriate for the numerical solution because of numerical instability of ill-posed problems. For this reason, the synthesis problem was only considered for low-density beams with no magnetic field when analytical solutions to Laplace's equation could be found using the theory of functions of a complex variable [6,7].

In order to overcome the complications, another approach was proposed in [8] that is based on the possibility of considering and solving numerically a series of more general well-posed boundary-value problems instead of a single problem arising due to the conventional approach. According to [8], some functions used for imposing the boundary conditions could be chosen arbitrarily so that a series of solutions for the electric and magnetic fields is obtained. In general, any of these could be used as the final solution since they all yield a solution to the original problem providing the required spatial structure of the beam.

The aim of this work is to develop the approach in [8] in order to find analytical solutions whenever possible and to propose the effective procedure for choosing the most appropriate solution for the electric and magnetic fields needed for preparing the dense laminar ion beams with a required spatial configuration.

II. PROBLEM FORMULATION

Consider a cylindrical focusing system of the length L and radius R supporting a dense laminar ion beam of axial symmetry and of gradually decreasing radius. The beam propagates along the z axis from the entrance plane at $z=0$ to the exit plane at $z=L$ and consists of one type of ion with mass m and charge e. The ions move within the beam due to the force of both the electric and magnetic fields, which are characterized by the scalar potential $U(r,z)$ and the vector potential $\boldsymbol{A}(r,z)=A_\varphi(r,z)\hat{\boldsymbol{\varphi}}$ with the axial symmetry of the system taken into account.

The ion trajectories are specified by their projections onto the meridional plane (r,z) in the cylindrical coordinate frame (r,φ,z),

$$r=r(r_0,z), \tag{1}$$

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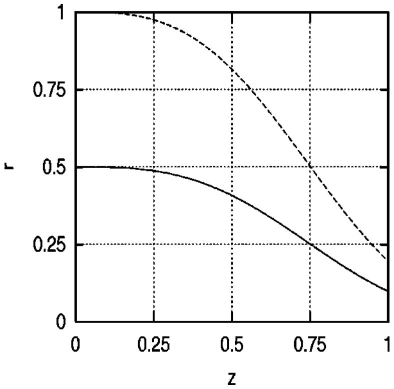

FIG. 1. Projections of the ion trajectories $r=r(r_0,z)$ onto the meridional plane (relative units).

where r_0 is the radial coordinate of the initial point $(r_0,0)$ of the trajectory considered (Fig. 1). For simplicity, we assume below that all the curves $r=r(r_0,z)$ are orthogonal to the r axis at $z=0$ and all the ions have the same axial velocity $V_z(r_0,0)=\mathrm{const}$ at the entrance plane $z=0$.

The density of the trajectories is specified by their radial distribution $p(r_0)$ at $z=0$. Using the condition $V_z(r_0,0)=\mathrm{const}$, the function $p(r_0)$ is normalized to be identical to the local ion density at the entrance plane, with $P_0=2\pi\int_0^R p(r_0)r_0 dr_0$ being the line density of the beam at $z=0$.

Notice that the ion trajectories in a laminar beam, although being twisted by the magnetic field, do not intersect, nor do their projections on the meridional plane given by Eq. (1). So, for any trajectory passing through any given point (r,z), a unique value for the initial coordinate $r_0=r_0(r,z)$ can always be found by inverting the functions (1).

Functions (1) should satisfy Stormer's trajectory equation [7]

$$\frac{d^2r}{dz^2}=\left(\frac{\partial Q}{\partial r}-\frac{\partial Q}{\partial z}\frac{dr}{dz}\right)\left[1+\left(\frac{dr}{dz}\right)^2\right]\frac{1}{2Q}, \tag{2}$$

where

$$Q=Q(r,z)=T-\eta(\Psi-\Psi_0)^2/r^2 \tag{3}$$

is the effective potential,

$$T=T(r,z)=-eU/|e|, \tag{4}$$

$\eta=|e|/(8\pi^2 m)$, $\Psi=\Psi(r,z)=2\pi r A_\varphi(r,z)$ is the magnetic flux associated with the circular loop of the radius r at the plane z, and $\Psi_0=\Psi_0(r_0)=\Psi(r_0,0)$ is the value of Ψ at the initial point $(r_0,0)$ of the trajectory passing through the point (r,z), with $r_0=r_0(r,z)$ according to Eq. (1).

The equivalent potential $Q(r,z)$ must be positive to determine the axial component of the ion velocity

$$V_z(r,z)=\sqrt{2|e|Q(r,z)/\{m[1+(dr/dz)^2]\}}. \tag{5}$$

$Q(r,z)$ should also satisfy the assumption $V_z(r_0,0)=\mathrm{const}$ made about the ion motion in Eq. (1).

Equation (2) is normally used to find the ion trajectories when $Q(r,z)$ is known. However, if the trajectories are known, one can use Eq. (2) to obtain the effective potential $Q(r,z)$. In terms of Q, Eq. (2) is a linear partial differential equation of the first order. Therefore, one can always solve it by the method of characteristics provided the trajectories have no return points and the boundary values of $Q(r,z)$ are given along the curve that is not a characteristic [9]. A suitable curve of this kind is the axis OZ, where the values $Q_0(z)=Q(0,z)$ determine the ion velocity along the axis,

$$V_0(z)=V_z(0,z)=\sqrt{2|e|Q_0(z)/m}. \tag{6}$$

The function $Q_0(z)$ is one of a series of functions chosen arbitrarily according to the approach in [8].

Once $Q(r,z)$ is found, the electric potential $U(r,z)=-|e|T(r,z)/e$ can be obtained from Poisson's equation,

$$\frac{\partial^2 U}{\partial r^2}+\frac{1}{r}\frac{\partial U}{\partial r}+\frac{\partial^2 U}{\partial z^2}=-\frac{\rho}{\varepsilon_0}, \tag{7}$$

where $\rho(r,z)$ is the space-charge density of the beam and ε_0 is the absolute permittivity. The function $\rho(r,z)$ is already available since it is determined by the ion trajectories $r(r_0,z)$, their entrance distribution $p(r_0)$, and the ion velocity $V_z(r,z)$, so that

$$\rho(r,z)=ep(r_0)(r_0/r)^2V_z(0,0)/V_z(r,z), \tag{8}$$

where $r_0=r_0(r,z)$ according to Eq. (1).

Equation (7) can be solved by any numerical method provided a well-posed boundary-value problem is formulated. A suitable formulation would be the Dirichlet problem when the functions $U(0,z)$, $U(R,z)$, $U(r,0)$, and $U(r,L)$ are considered as the given boundary values required for the unique solution $U(r,z)$ to be obtained. These functions can be freely chosen to be any reasonably smooth functions.

Proceeding in this way, one obtains the function $T(r,z)=-eU(r,z)/|e|$, which is normally different from the function $Q(r,z)$. This means that some magnetic field is generally required to obtain the desired trajectories (1). The magnetic field can be found from the magnetic flux $\Psi(r,z)$ calculated as

$$\Psi(r,z)=\Psi_0(r_0)+r\sqrt{(T-Q)/\eta}, \tag{9}$$

where $\Psi_0(r_0)=\Psi(r_0,0)$ is also the function chosen arbitrarily and $r_0=r_0(r,z)$.

Thus, according to this approach, an infinite set of various solutions for the electric and magnetic fields can be found depending on a few arbitrarily chosen functions, and each of the solutions provides the same set of the trajectory projections $r=r(r_0,z)$ on the meridional plane as required, although the trajectories can be twisted in a different way about the beam axis.

Notice, however, that the choice of some arbitrary functions is in some aspects restricted. First, according to the definition of Q, one has always the condition

$$T(r,0)=Q(r,0) \tag{10}$$

but this only implies that the total number of arbitrary functions is less by just one [the boundary value $U(r,0)$ is determined by the solution $Q(r,0)$].

Next, the solution $Q(r,z)$ must be positive as discussed above because of the definition of Eq. (5). Typically, it appears that for the positive function $Q_0(z)$, the solution $Q(r,z)$ is also positive, as in the example considered below [the other requirement, $V_z(r_0,0)=\text{const}$, is also satisfied in this example].

Further, the functions $Q(r,z)$ and $T(r,z)$ should satisfy the condition

$$Q(r,z)-T(r,z)<0 \tag{11}$$

according to the definition of Q, Eqs. (3) and (9). This is a rather serious restriction, but in practice a free choice of the whole set of other functions still allows quite enough space for playing with various solutions, each of which provides the same set of curves $r=r(r_0,z)$ on the meridional plane, so that the restriction can be rather loose in many cases (such a case is considered in the next section).

Finally, there is another kind of restriction concerning the behavior of the potentials Q and U as functions of r near the beam axis. The matter is that, assuming no electric charge of δ-function density is placed at the axis, one has the electric potential satisfying the condition

$$\left.\frac{\partial U}{\partial r}\right|_{r=0}=0. \tag{12}$$

On the other hand, when the magnetic field does not increase very fast near the axis, i.e., when $B_z\sim o(r^{-1})$ at $r\rightarrow 0$, one has $\Psi(r,z)\sim o(r)$, $r\rightarrow 0$, so that another condition arises, $U(0,z)=-eQ(0,z)/|e|$, i.e.,

$$T(0,z)=Q(0,z), \tag{13}$$

where $Q(0,z)=Q_0(z)$ is the boundary function used in Eq. (2).

The conditions (12) and (13) are quite crucial. In fact, it is due to these requirements used as the only boundary conditions for Eq. (7) that the ill-posed Cauchy problem for Laplace's equation arises in the conventional approach when the beam charge is neglected [7]. In such a formulation, the given problem is numerically unstable and as a result the whole approach is inappropriate for numerical simulation.

Notice, however, that neither condition (12) nor (13) is formally required from the more general point of view, and so neither one is a nominal restriction. Violation of these conditions means only either imposing a fixed line charge at the Z axis or increasing magnetic field too rapidly when $r\rightarrow 0$, respectively. Nevertheless, satisfying both the conditions (12) and (13) is, indeed, necessary from the practical point of view. Therefore, a method that allows these complications to be overcome by means of a more general analysis is needed.

A simple iterative procedure for solving this problem by satisfying both conditions (12) and (13) simultaneously when performing numerical calculations is proposed in the next section of the paper. At the same time, it appears that condition (11) is also better satisfied as a result of such iterations.

III. NUMERICAL RESULTS

Let us apply the approach considered above to the case when the ion trajectories $r(r_0,z)$ and their transverse distribution $p(r_0)$ at the entrance plane are given by the functions

$$r(r_0,z)=r_0\exp[-(z/f)^3] \tag{14}$$

and

$$p(r_0)=\frac{P_0}{\pi a^2}\exp[-(r_0/a)^2], \tag{15}$$

where f is the effective focal length, a is the entrance beam radius, and P_0 is the line density of the beam at the entrance plane $z=0$.

The functions (14) are very suitable for the analysis since, first, they allow us to find an analytical solution to Eq. (2), second, they describe a significant compression of the ion beam (Fig. 1), and third, they correspond to the case when the plane $z=0$ is an equipotential surface that can be considered as a planar surface of the ion emitter.

As one can see, since both the first and second derivatives of the functions $r(r_0,z)$ with respect to z are zero at $z=0$, the curves $r(r_0,z)$ are normal to the r axis at $z=0$ and the requirement of $V_z(r_0,0)=\text{const}$ is also automatically satisfied [see Eq. (3)].

In the case considered, Eq. (2) takes the form

$$\frac{\partial Q}{\partial r}+\frac{3rz^2}{f^3}\frac{\partial Q}{\partial z}=-6rz\frac{2f^3-3z^3}{f^6+9r^2z^4}Q. \tag{16}$$

This has an analytical solution

$$Q(r,z)=Q_0(z_0)\frac{1+9r^2z^4/f^6}{(1+3r^2z/2f^3)^4}, \tag{17}$$

where $Q_0(z_0)$ is the boundary-value function chosen arbitrary, with the value z_0 being defined as $z_0=z/(1+3r^2z/2f^3)$. The solution $Q(r,z)$ is positive everywhere at $z\geqslant 0$ if the axial boundary function $Q_0(z_0)$ is chosen positive as required by definition of both $Q(r,z)$ and $Q_0(z_0)$, Eqs. (5) and (6).

Now, taking some functions $Q_0(z_0)>0$, $U(R,z)$, and $U(r,L)$, and imposing boundary conditions (10) and (12) or (10) and (13), one can solve Eq. (7) by any numerical method (the efficient method based on Stone's strongly implicit procedure [10] has been used in this work). In this manner, one generally obtains a kind of solution that does not satisfy Eq. (13) or Eq. (12), respectively, and often does not satisfy condition (11) either.

In order to get a solution that satisfies all the required conditions, the following iterative procedure was implemented. First, starting from any reasonable function $Q_0(z_0)>0$ and imposing the condition (12), one obtains a solution $U(r,z)$ with $T(0,z)\neq Q_0(z)$. Then, the function $Q_0(z)$ is updated to be equal to the function $T(0,z)$ just obtained. Now, the new function $Q_0(z)$ is used as the axial boundary function in Eq. (17) and the solution $U(r,z)$ is updated, always assuming the condition (12). In this way, the iterations continue until the required solution is obtained.

The iterations appear to be convergent providing the final solution $Q_0(z)$, $Q(r,z)$, and $T(r,z)$, which satisfy both the conditions (12) and (13) simultaneously. Moreover, there is a domain of the parameters where the condition (11) is also satisfied, despite the tendency to be violated for the beams of higher density and compression.

Some examples of the solutions obtained in this way for the beam specified by Eqs. (14) and (15) are discussed below. The solutions are found for two similar systems that differ only by the boundary conditions at the side wall $r=R$ and at the exit plane $z=L$. The boundary conditions common for both systems, in addition to Eqs. (10), (12), and (13), are

$$\Psi_0(r_0)=0 \quad \text{at} \quad 0\leqslant r\leqslant R, \quad z=0, \tag{18}$$

$$\partial T(r,z)/\partial z=0 \quad \text{at} \quad 0\leqslant r<r_1, \quad z=L, \tag{19}$$

and

$$T(r,z)=T_L \quad \text{at} \quad r_1\leqslant r\leqslant r_2, \quad z=L, \tag{20}$$

where $T_L=-|e|U_L/e$ is the given potential of the ring-shaped counterelectrode (collector) at the exit plane $z=L$. The potential at the entrance plane, $T_0=T(r,0)$, related to the ion velocity $V_z(r,0)$ by Eqs. (5) and (10), is not specified, being determined self-consistently by the solution $Q(r,z)$.

The other boundary conditions, specific in each case, are

$$\begin{aligned} &T(R,z)=Q(R,z), \quad 0\leqslant z\leqslant L,\\ &T(r,L)=Q(r,L), \quad r_2<r\leqslant R \end{aligned} \tag{21}$$

for the first system and

$$\begin{aligned} &T(R,z)=T_0, \quad 0\leqslant z\leqslant L,\\ &\partial T(r,L)/\partial r=0, \quad r_2<r\leqslant R \end{aligned} \tag{22}$$

for the second one.

In the first case, the conditions (18) and (21) require that the magnetic flux through the circular loops at the relevant boundaries [e.g., $\Psi(R,z)$ when $r=R$, $0\leqslant z\leqslant L$] should be zero while the potential should vary properly between the emitter and the collector, with the emitter being the entrance plane $z=0$. In the second case, no conditions are imposed on the magnetic flux on the boundaries $r=R$ and $z=L$, with the only typical requirement of zero flux at the emitter [7], Eq. (18). In this case, however, the side walls should be maintained at the potential of the emitter.

Solutions for the first system are shown in Figs. 2 and 3, where the parameters, in relative units, are $L=1$, $R=1$, $f=0.85$, $a=0.5$, $r_1=0.125$, $r_2=0.375$, and $T_L=1$, with $P_0=2$ [Fig. 2(a)] and $P_0=0.1$ [Fig. 2(b)] for the beam of high and low density, respectively. For the values $L=1$ cm and $T_L=10$ kV, in the case of an electron beam

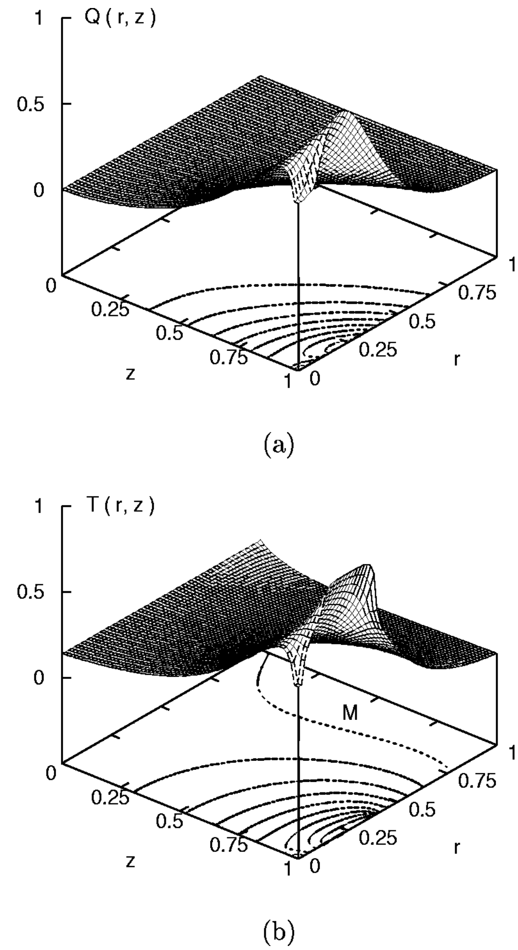

FIG. 2. The solutions (a) $Q(r,z)$ and (b) $T(r,z)$ found for the first focusing system (relative units).

($m=m_e$) with $P_0=2$, it corresponds to $Q_0(0)=37$ V, $Q_0(L)=4.75$ kV, $V_0(0)=3.6\times10^8$ cm/s, and $V_0(L)=4\times10^9$ cm/s. Such a system would focus a laminar beam carrying a total current $I_e=0.63$ A, with the entrance and exit beam radii $a_0=5$ mm and $a_L=1$ mm that correspond to the mean current densities $j_0=0.8$ A/cm^2 and $j_L=20$ A/cm^2, respectively, and to the maximum electron density at the exit plane $n_{\max}=n(0,L)=3\times10^{10}$ 1/cm^3 (the ion beam would be of the same density, with the current $I=I_e\sqrt{m_e/m}$).

The shape of the function $Q(r,z)$, Fig. 2(a), is rather typical for various kinds of boundary conditions, including the cases in which $T(r,L)=Q(r,L)$ at the whole collector plane $z=L$ $(0\leqslant r\leqslant R)$ or, e.g., when $T(r,L)=T_L$ at $0\leqslant r\leqslant R$ and $T(R,z)=T_0+(T_L-T_0)z/L$ at $0\leqslant z\leqslant L$. The reason is that $Q(r,z)$ is defined via the ion velocity on axis, Eq. (6), established self-consistently together with the space-charge distribution, which is quite a robust entity.

The typical shape of $Q(r,z)$ determines the optimum size and position of the collector as specified above, which allows us to satisfy condition (11) in all the cases considered. With such a collector, the potential function $T(r,z)$ is also rather typical, except for minor features like the one observed in Fig. 2(b) for the low-density beam of $P_0=0.1$, which is quite

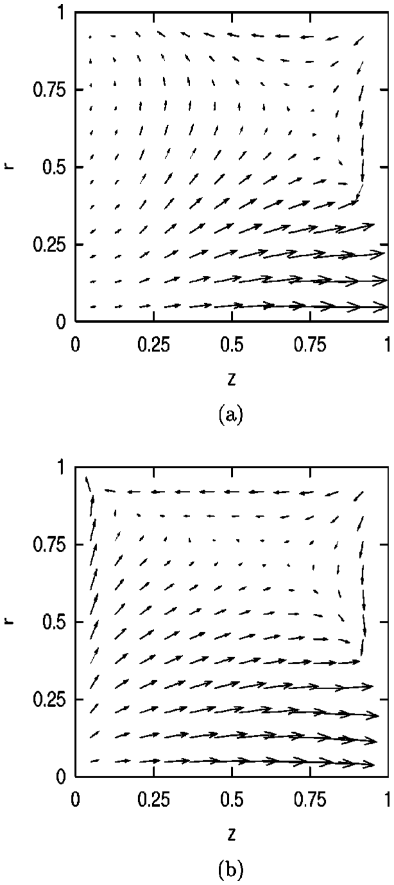

FIG. 3. The magnetic flux $\Psi(r,z)$ required for supporting the beam of (a) high and (b) low density in the first focusing system (relative units).

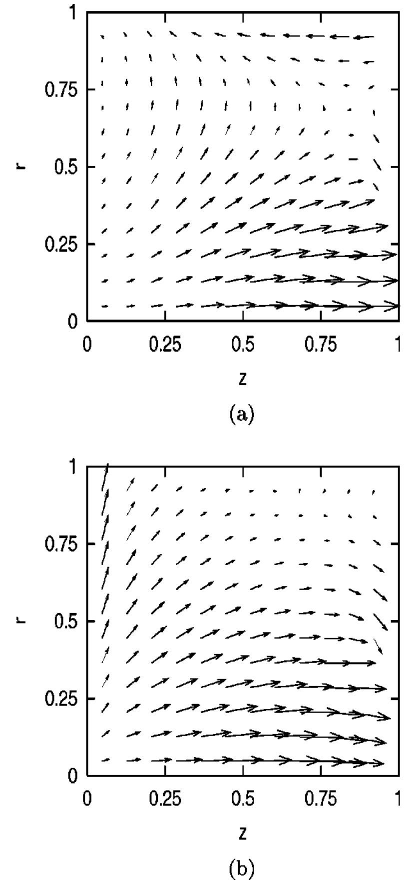

FIG. 4. The magnetic flux $\Psi(r,z)$ required for supporting the beam of (a) high and (b) low density in the second focusing system (relative units).

close to the limiting case of $P_0=0$. In this case, an additional electrode at the side wall would be useful (e.g., the one coinciding with the equipotential curve M at a slightly repulsive potential $T_M=0.1$ compared to the potential of the emitter $T_0=0.14$) in order to improve the distribution of $T(r,z)$ near the wall.

Magnetic field is more sensitive to the choice of boundary conditions since it depends on the difference of two functions, $Q(r,z)$ and $T(r,z)$. Figures 3(a) and 3(b) show the magnetic field $\vec{B}(r,z)(|B_{\max}|\sim 0.2\ \mathrm{T})$ needed for supporting the beams of high and low density, respectively.

Solutions for the second focusing system producing a dense beam are similar to the ones shown above, especially in the region occupied by the beam. The distinction, however, increases for beams of lower density [cf. Figs. 3, 4(a), and 4(b), respectively] since the fields inside the beam become more sensitive to the boundary conditions when the space charge of the beam decreases.

In general, the second system is much simpler compared to the first one, both in the design of the side-wall electrode (now it is just a cylindrical continuation of the emitter at $r=R$ and $0\leqslant z\leqslant L$) and in the distribution of the magnetic field, Figs. 4(a) and 4(b). At the same time, creating the particular distribution of the magnetic field as defined by the solutions of Eqs. (2) and (7) is crucial for producing the perfect laminar beam of the given density and spatial configuration.

For comparing different solutions discussed above, Fig. 5 shows the ion velocity on the beam axis. Lower values of the velocity at the emitter observed for the beams of higher density at the same value of T_L are a result of a significant space charge accumulated in the beam. The latter prevents the ions from being properly accelerated and, with further increasing the beam density, disrupts the laminar ion motion so that no solution can be obtained for the given trajectories at the given values of the parameters.

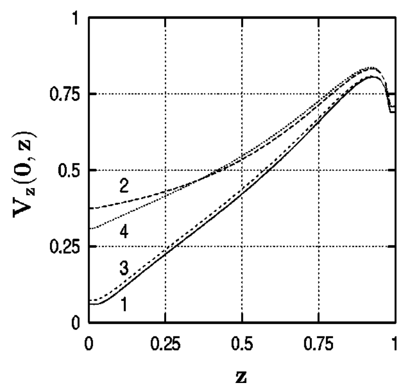

FIG. 5. Ion velocity on the beam axis, $V_z(0,z)$, found self-consistently for the beams of high (1,3) and low (2,4) density in the first (1,2) and in the second (3,4) focusing systems (relative units).

Because of such an effect, the solutions for the dense beam found above are, in fact, nearly at the highest values for the system parameters that determine the density and the rate of compression of the laminar beam (P_0, f, and L at the fixed values of R and T_L) for the given set of the ion trajectories. This example, however, is much too restrictive because of the extremely fast convergence of the trajectories required by Eq. (1). With more realistic sets of trajectories converging into a dense beam not so rapidly (such as in the Pierce gun [11], etc.), a solution may exist for the beams of a higher density, although in these cases one may need to solve Eq. (2) numerically as explained in [8].

IV. CONCLUSIONS

In this work, we have shown that the problem of numerical synthesis of ion-beam focusing systems that prepare dense laminar beams of a given profile and compression can be reduced to successive solutions of two well-posed boundary-value problems for the linear partial differential equations, instead of the ill-posed problem arising due to the conventional approach when the space charge of the beam is neglected.

According to the new approach, the first problem to solve is Stormer's trajectory equation formulated in terms of the unknown equivalent potential Q. An analytical solution to this equation for a specific kind of focusing system has been found.

The second problem is to obtain the proper solution of Poisson's equation. Well-posed boundary-value problems have been considered in order to obtain such a solution. A self-consistent numerical method for satisfying the axial boundary conditions for Poisson's equation is proposed.

Analytical solutions and numerical simulations have shown that, generally, the required dense laminar ion beam with the ion trajectories of a desired profile can be formed by the proper superposition of both the electric and magnetic fields, despite the tendency of the magnetic field to mix the trajectories.

In general, the beams of the same shape can be formed by essentially different electric and magnetic fields depending on the choice of a few arbitrary functions used as the boundary conditions. Some examples of the solutions of this kind have been provided.

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