ANALYTICAL PRESENTATION OF SPACE CHARGE FORCES*

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Abstract

This paper presents an analytical description of space charge forces generated by charged particle beams. Suggested approach is based on some set of models for particle distribution function. All necessary calculations have analytical and closed form for different models for beam density distributions. These model distributions can be used for approximation of real beam distributions. The corresponding solutions are included in general scheme of beam dynamics presentation based on matrix formalism for Lie algebraic tools. Computer software is based on corresponding symbolic codes and some parallel technologies. In particular, as computational tools we consider GPU graphic card NVIDIA. As an example, we consider a problem of beam dynamics modelling for microprobe focusing systems.

INTRODUCTION

Most of space charge modelling methods are based on numerical methods and corresponding programming technologies. In particular, matrix processors became very popular in the last time for numerical evaluations (i. e. using the Particle-in-Cell method). But for long time beam evolution problems these methods demonstrate rather low effectiveness. The nature of the corresponding beam dynamics needs effective algorithms for space charge field reconstruction during the beam evolution along the reference orbit (with coordinate s). For this purpose in this paper we consider the following two methods: a beam with elliptical form in transverse four-dimensional phase space (*unbunched beam model*) and a beam presented as six-dimensional ellipses (*bunched beam model*). For the both models we use Ferrer's integrals method [1]. This method allows to derive corresponding formulae for beam generated field in symbolic forms. Similar presentation is compatible with presentation of the corresponding beam dynamics using Lie algebraic tools formalism [2]. In this paper we demonstrate evaluation method of electrical field generated by different distribution functions of beam particles. The analytical presentation of corresponding solutions is matched with matrix formalism for Lie algebraic tools [3]. Furthermore this approach can be realized for solution of Maxwell–Vlasov equations [4].

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DISTRIBUTION FUNCTION IN PHASE SPACE

In this section we demonstrate basic idea of our approach using the first models – the unbunched beam model in four-dimensional space with following coordinates $\{x, p_x, y, p_y\}$. The corresponding distribution function $f(x, p_x, y, p_y, s)$ can be presented as a function of $\varkappa^2 = \mathbf{X}^{\mathrm{T}}\mathbb{A}\mathbf{X}$, where $\mathbf{X} = (x, y, p_x, p_y)^{\mathrm{T}}$ and $\mathbb{A}$ is a symmetric nonsingular matrix. Let us consider some popular functions to present space charge distribution.

1) *Uniform distribution*:

$$\varphi(\varkappa^2) = \frac{2\sqrt{\det\mathbb{A}}}{\pi^2}\Theta(1-\varkappa^2),\ \Theta(x) = \begin{cases}1, & x \geq 0,\\ 0, & x < 0.\end{cases}$$

2) *Vladimirov–Kapchinsky* (*microcanonical*) *distribution*:

$$\varphi(\varkappa^2) = \frac{\sqrt{\det\mathbb{A}}}{\pi^2}\delta(1-\varkappa^2).$$

3) *Normal* (*Gauss*) *distribution*:

$$\varphi(\varkappa^2) = \frac{\sqrt{\det\mathbb{A}}}{4\pi^2}\exp\left(-\frac{\varkappa^2}{2}\right).$$

Of course, three indicated types of distributions don't exhaust all variety of admissible distributions family. But these distributions are interesting from point of view of configuration distributions of charge density in the configuration space (in the next we omit the variable s for reduction).

$$\rho(x, y) = \int\limits_{R^2} f(x, p_x, y, p_y)\, dp_x\, dp_y.$$

Indeed, practically, it is very difficult to measure the function $f(\mathbf{X})$, but the distribution $\rho(x, y)$ can be obtained with measurement accuracy. More over, only function $\rho(x, y)$ defines the electrical potential (or electrical field) which is necessary for beam dynamics evaluation. Let present the matrix $\mathbb{A}$ in a block matrix form

$$\mathbb{A} = \begin{pmatrix}\mathbb{A}^{11} & \mathbb{A}^{12}\\ \mathbb{A}^{21} & \mathbb{A}^{22},\end{pmatrix},\quad \mathbb{A}^{kk} = \left(\mathbb{A}^{kk}\right)^{\mathrm{T}},\ \ \mathbb{A}^{21} = \left(\mathbb{A}^{12}\right)^{\mathrm{T}},$$

then we can write

$$\varkappa^2 = \mathbf{X}^{\mathrm{T}}\mathbb{A}\mathbf{X} = \mathbf{X}_1^{\mathrm{T}}\mathbb{A}^{11}\mathbf{X}_1 + \mathbf{X}_1^{\mathrm{T}}\mathbb{A}^{12}\mathbf{X}_2 + \\ + \mathbf{X}_2^{\mathrm{T}}\mathbb{A}^{21}\mathbf{X}_1 + \mathbf{X}_2^{\mathrm{T}}\mathbb{A}^{22}\mathbf{X}_2,$$

where $\mathbf{X}_1 = (x, y)^{\mathrm{T}}$, $\mathbf{X}_2 = (p_x, p_y)^{\mathrm{T}}$. After some evaluations one can obtain the following equalities.

1) *Uniform distribution*:

$$\rho(x, y) = \frac{2qN_0}{\pi}\sqrt{\frac{\det\mathbb{A}}{\det\mathbb{A}^{22}}}(1-\varkappa_r^2)\Theta(1-\varkappa_r^2),$$

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where $\varkappa_r^2 = \mathbf{X}_1^{\mathrm{T}}\mathbb{C}\mathbf{X}_1$, $\mathbb{C} = \mathbb{A}^{11} - \mathbb{A}^{21}\left(\mathbb{A}^{22}\right)^{-1}\mathbb{A}^{12}$.
2) KV-*distribution*:

$$\rho(x,y) = \frac{qN_0}{\pi}\sqrt{\frac{\det\mathbb{A}}{\det\mathbb{A}^{22}}}\delta(1-\varkappa_r^2).$$

3) *Gauss-distribution*:

$$\rho(x,y) = \frac{qN_0}{2\pi}\sqrt{\frac{\det\mathbb{A}}{\det\mathbb{A}^{22}}}\exp\left(-\frac{\varkappa_r^2}{2}\right).$$

Where q – a particle charge, N_0 – a number of particle in transverse section.

For our long beam model we have $I(s,t) = v_0\int_{R^2}\rho(x,y,s,t)dxdy = \text{const}$, where v_0 – a longitudinal particle velocity. For definition of the matrices $\mathbb{A}^{ik}$ and $\mathbb{C}$ we impose some natural conditions: 1) $v_0\int_{R^2}\rho_i(x,y)\,dx\,dy = I = \text{const}$, $\forall\, i = \overline{1,3}$; 2) $\rho_i(0,0) = \rho_0$. As reference values we choose corresponding values for KV-distribution (the case of an "ideal beam")

$$\rho_0 = \frac{qN_0}{\pi}\sqrt{\frac{\det\mathbb{A}}{\mathbb{A}^{22}}},\quad I = v_0 qN_0\sqrt{\frac{\det\mathbb{A}}{\det\mathbb{A}^{22}}\det\mathbb{C}}\ .$$

Excepting N_0 one evaluates $\rho_0 = I\sqrt{\det\mathbb{C}}/\pi v_0$.

The matrix $\mathbb{C}_i$ describes the ellipse for the i-th case, we can suppose $\mathbb{C}_i = \alpha_i^2\mathbb{C}$, that is we consider as an ellipse. Then 2), 3) can be rewritten in the form

$$\rho_1(x,y) = \rho_0(1-\alpha_1^2\varkappa^2)\Theta(1-\alpha_1^2\varkappa^2),$$
$$\rho_2(x,y) = \rho_0\Theta(1-\alpha_2^2\varkappa^2),\quad \rho_3(x,y) = \rho_0\exp(-\alpha_3^2\varkappa^2),$$

where $\varkappa^2 = \mathbf{X}_1^{\mathrm{T}}\mathbb{C}\mathbf{X}_1$, $\mathbb{C}$ – a matrix describing an ellipse in configuration space for the ideal beam. The second condition for definition of our free parameters we get from the equality $\rho_1 = \rho_2$. After some simple evaluations we get $\alpha_1 = 2/3$ and $\alpha_2 = 1$. It means that function ρ_1 leads to the same value as homogeneous distribution ρ_2, if it be defined for ellipse $X_1^{\mathrm{T}}\mathbb{C}X_1 \le 9/4$. Analogical evaluations can be performed for any distributions. We should note that function $\rho_3(x,y)$ has not a compact support. For similar distributions we should define the probability for ingressing to the interior of ellipse $\mathbf{X}_1^{\mathrm{T}}\mathbb{C}\mathbf{X}_1 \le \lambda^2$. Here λ^2 defines a "beam boundary" with some probability. For example, for probability $P = 0.9$ we obtain $\alpha_3 = 9/\left(5\sqrt{\pi}\,\mathrm{erf}(1)\right)$ and $\lambda = 1/\alpha_3$.

Besides the mentioned distributions we point the following two distribution: quadratic – $\rho_4(x,y) = \rho_0(1-\alpha_4^4\varkappa^4)\Theta(1-\alpha_4^2\varkappa^4)$ and cosine-like – $\rho_5(x,y) = \rho_0\cos^2(\alpha_5^2\varkappa^2)\Theta(1-\varkappa^4/2)$. Like in previous cases we can evaluate α_4 and α_5 (this coefficient evaluates via known Fresnel function). We should note that described types of modelling functions (both in phase and in configuration spaces) demonstrate the suggested approach, which can be used practically for any distribution function. In particular, one can use instead of the function $\rho(x,y)$ a polynomial of quadratic form variable $\varkappa^2$ with some polynomial order agreed with known nonlinear order for control electromagnetical fields. As an additional step we can suggest the method of Padé approximation, which makes possible to select corresponding coefficients with desired accuracy.

SELF-FIELD OF SPACE CHARGE

For many practical problems of beam physics we can suggest that phase space distribution function $f(\mathbf{X})$ and configuration distribution function ρ are functions of transverse coordinates only. In other words $f = f(\mathbf{X})$ and $\rho = \rho(x,y)$ for some small interval of variable s. In this case Poisson equation for electrical potential Ψ (inside the beam ellipsoid), can be written in form

$$\frac{\partial^2\Psi}{\partial x^2} + \frac{\partial^2\Psi}{\partial y^2} = -\frac{1}{\varepsilon_0}\rho(x,y). \quad (1)$$

According to the first section we assume $\rho(x,y) = \rho_0\varphi(\varkappa^2)$, where φ – certain function (e. g. one of pointed five functions) of argument $\varkappa^2 = \mathbf{X}_1^{\mathrm{T}}\mathbb{C}\mathbf{X}_1$, $\mathbf{X}_1 = (x,y)^{\mathrm{T}}$. For small enough interval Δs the resulting essential variation of ellipse axes can be negligible. So, in coordinates (ξ,η) the ellipse will be canonical: $\varkappa^2 = \xi^2/a^2 + \eta^2/b^2$. We need to use elliptic coordinates $\xi = h\cosh\alpha\cos\beta$, $\eta = h\sinh\alpha\sin\beta$ to solve (1). Poisson equation transforms to the following form

$$\frac{\xi^2}{\alpha^2} + \frac{\eta^2}{\beta^2} = -\frac{1}{\varepsilon_0}\rho h^2\left(\cosh^2\alpha - \cos^2\beta\right),$$

with solution in coordinates ξ, η:

$$\Psi(\xi,\eta) = -\frac{1}{4\varepsilon_0}\rho\left(\xi^2+\eta^2 - \frac{a-b}{a+b}\left(\xi^2-\eta^2\right)\right) + \Psi_0,$$

or finally in coordinates x, y:

$$\Psi(x,y) = -\frac{1}{4\varepsilon_0}\rho\left(x^2+y^2 - \right.$$
$$\left. - \frac{a-b}{a+b}\left(x^2\cos 2\gamma - y^2\cos 2\gamma + 2xy\sin 2\gamma\right)\right) + \Psi_0,$$

where $\gamma = \arctan\left(2c_{12}/(c_{22}-c_{11})\right)$ – the rotation angle for coordinates transformation with rotation matrix $\mathbb{T}$.

Let consider the known approach based on Ferrer's integral [1]. According to this approach we obtain for inner potential of elliptic cylinder

$$\Psi^{(i)} = -\frac{\pi ab}{eps_0}\int\limits_0^\infty \Phi\left(\varkappa^2(u)\right)\frac{du}{\Delta(u)},$$

where $\Phi(\varkappa^2) = \int_0^{\varkappa^2}\rho(t)dt$, $\Delta^2(u) = (a^2+u)(b^2+u)$, $\varkappa^2(u) = \xi^2/(a^2+u) + \eta^2/(b^2+u)$. One can obtain electrical field generated by space charge

$$E_\xi^{(i)}(\xi,\eta) = \frac{2\pi ab}{\varepsilon_0}\int\limits_0^\infty \frac{\xi}{a^2+u}\rho\left(\varkappa^2(u)\right)\frac{du}{\Delta(u)},$$

$$E_\eta^{(i)}(\xi,\eta) = \frac{2\pi ab}{\varepsilon_0}\int\limits_0^\infty \frac{\eta}{b^2+u}\rho\left(\varkappa^2(u)\right)\frac{du}{\Delta(u)}.$$

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On the next step we evaluate components of the electrical field E_ξ, E_η for our charge distribution functions. Using inverse transformation $\mathbb{T}^{-1}$ we can obtain E_x, E_y (electrical field components in initial coordinate system). After some evaluations one can determine (using Euler substitution $t = \Delta(u)/(a^2+u)$, $u = b^2 - a^2t^2/(t^2-1)$, $t(0) = b/a$, $t(\infty) = 1$):

$$E_\xi = \frac{4\pi\rho_0}{\varepsilon_0}\frac{ab}{a(a+b)}\xi, \quad E_\eta = \frac{4\pi\rho_0}{\varepsilon_0}\frac{ab}{b(a+b)}\eta.$$

We will denote it as E^0_ξ and E^0_η. For the linear distribution in $\varkappa^2$ we obtain for the components of electrical field correspondingly

$$E_{\xi,\eta} = E^0_{\xi,\eta} + \Delta E_{\xi,\eta}, \tag{2}$$

$$\Delta E_\xi = -\frac{4\pi\rho_0}{\varepsilon_0}\frac{a_1b_1}{a_1^2+b_1^2}\xi\left(\frac{2a_1+b_1}{3a_1^3}\xi^2 + \frac{1}{a_1b_1}\eta^2\right),$$
$$\Delta E_\eta = -\frac{4\pi\rho_0}{\varepsilon_0}\frac{a_1b_1}{a_1^2+b_1^2}\eta\left(\frac{1}{a_1b_1}\xi^2 + \frac{2b_1+a_1}{3b_1^3}\eta^2\right).$$

The described approach can be used for all of our distributions. We obtain formulae similar to (2) with corresponding expressions for $\Delta E_{\xi,\eta}$.

After rotation for Gauss distribution $\rho_3(x,y) = \rho_0\exp\left(-\varkappa^2\right)$ we have $\varkappa^2 = \xi^2/a^2 + \eta^2/b^2 \le 1$. Using the Euler substitution and integration on ξ, η we can obtain

$$E_{\xi,\eta} = E^0_{\xi,\eta} + \Delta E_{\xi,\eta},$$

$$\Delta E_\xi = -\frac{4\pi\rho_0}{\varepsilon_0}ab\xi\left[\exp\left(\frac{\xi^2-\eta^2}{b^2-a^2}\right)-1\right]\times$$
$$\times\sum_{k=1}^{\infty}\left[\chi^1_k\left(\frac{\eta}{\xi}\right) - \left(\frac{b}{a}\right)^{2k+1}\chi^1_k\left(\frac{\eta a^2}{\xi b^2}\right)\right],$$
$$\Delta E_\eta = -\frac{4\pi\rho_0}{\varepsilon_0}ab\xi\left[\exp\left(\frac{\eta^2-\eta^2}{b^2-a^2}\right)-1\right]\times$$
$$\times\sum_{k=1}^{\infty}\left[\chi^2_k\left(\frac{\eta}{\xi}\right) - \left(\frac{b}{a}\right)^{2k-1}\chi^2_k\left(\frac{\eta a^2}{\xi b^2}\right)\right],$$

where $\chi^1_k(x) = \frac{\xi^{2k}}{k!(b^2-a^2)^{k+1}}\sum_{j=0}^{k}\frac{(-1)^{k-j}C^j_k}{2k+1-4j}x^{2j}$, $\chi^2_k(x) = \frac{\xi^{2k}}{k!(b^2-a^2)^{k+1}}\sum_{j=0}^{k}\frac{(-1)^{k-j}C^j_k}{2k-1-4j}x^{2j}$. For distributions $\rho_4(x,y) = \rho_0(1-4\varkappa^4/9)\Theta(1-4\varkappa^4/9)$ and $\rho_5(x,y) = \rho\cos^2(\varkappa^2\frac{\pi}{4})\Theta(2-\varkappa^2)$ rotation and scaling lead to $\rho_5(\xi,\eta) = \cos^2(\pi\varkappa_5^2/2)\Theta(1-\varkappa_5^2)$, $\varkappa_5^2 = \xi^2/a_5^2+\eta_5^2/b_5^2 \le 1$, $a_5 = \sqrt{2}a$, $b_5 = \sqrt{2}b$ we also obtain the corresponding series.

We should note that any space charge distribution $\rho(x,y)$ with polynomial of n-order according $\varkappa^2$ leads us to polynomial $\Delta E_{\xi,\eta}$ order $2n+1$.

The above exemplified formulae can be essentially simplified for a circular beam ($a = b = R$). For example, for *Cosine-like distribution* we have:

$$\Delta E_\xi = \frac{2\pi\rho_0}{\varepsilon_0}\xi\left(\frac{2R^2}{\pi(\xi^2+\eta^2)}\sin\frac{\pi(\xi^2+\eta^2)}{2R^2}-1\right),$$
$$\Delta E_\eta = \frac{2\pi\rho_0}{\varepsilon_0}\eta\left(\frac{2R^2}{\pi(\xi^2+\eta^2)}\sin\frac{\pi(\xi^2+\eta^2)}{2R^2}-1\right).$$

After returning to the initial coordinate system we can obtain components $E_{x,y}$.

CONCLUSION – PARALLEL CALCULATIONS FOR BEAM DYNAMICS

In the previous sections we have considered methods which allow to evaluate a power series expansion for electrical field. The form of these series allows us to use matrix formalism for beam dynamics both in external (control) and self-field generated by beam [5]. The presentation of these fields in the same form allows us to use the method predictor-corrector for beam dynamics evaluation [6] for nonlinear fields also. The matrix presentation practically of all objects allows us to parallelize necessary operations. More over the necessary processors load it is not so essential as compared with parallelization of "usual" approach based on PIC or other similar methods. The computer simulation of some beam transport lines demonstrated necessary effectiveness of the described approach. The computation process divides into several levels of parallelization (parallelization tree) that allows us to constraint effective programs using GPU graphic card TESLA S2050, OpenCL and CUDA technologies [7].

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