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Numerical simulation of space charge effects in the sector cyclotron

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Abstract To study the effects of space charge in cyclotrons and synchrocyclotrons the code PHASCOL is developed. A method of large (macro)particles is realized in this code. The complete equations of motion of the charged particle in electromagnetic field of accelerator are integrated taking into account the three-dimensional self-electric field of beam. Two methods were used for the calculation of the beam field: the particle-to-particle method and the particle-in-cell one. The results of calculations which illustrate space-charge effects on the parameters of beam in the process of acceleration are given. Both methods have shown a similar influence of space charge on the beam.

Key words sector cyclotron • particle dynamics • space charge

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Introduction

To increase the intensity of the JINR synchrocyclotron from 5 to 50 μA, a project [3] of external injection of the beam of energy 5 MeV into the central region of accelerator is under design. One of the versions of injector is examined by 4-fold sector cyclotron with final energy of 5 MeV of H^- ions and an average beam current of 15–20 mA. At this intensity of beam, it is necessary to know detailed information about space-charge effects (SCE) on particle dynamics. Numerical simulations [1] that were done in PSI and are intended for two-dimensional SCE in the cyclotron with sectioned magnetic system are well known. We were faced with the task to fulfill three-dimensional SCE simulation with the minimum of simplifying assumptions.

To study SCE in cyclotrons and synchrocyclotrons, the code PHASCOL, in which is realised the method of large (macro)particles, is created. To be more sure of the validity of the obtained results, two methods were used for calculating self field of the beam: the method of pairwise interactions and the method of particle in cell. In the first method, electric field in the location of the macroparticle is calculated by summing up the Coulomb's field, which acts from the side of the remaining particles. In the second method, with the aid of rapid Fourier's transform the three-dimensional Poisson's equation on the grid, which covers beam, is solved numerically.

Brief description of the code PHASCOL

Equations of motion

For numerical simulation of the effects of space charge, the beam is subdivided into a series of the bunches injected into the accelerator, each of them consisting of a set of particles. The sum charge of the particles corresponds to the beam current being simulated. The following complete equations of motion [6] of the charged particle in the cylindrical coordinate system are used in PHASCOL:

$$(1)\quad \ddot{r} = r\dot{\varphi}^2 + \frac{qc^2}{E}\left[\varepsilon_r - r\dot{\varphi}B_z + \dot{z}B_\varphi - \frac{\dot{r}}{c^2}\left(\dot{r}\varepsilon_r + r\dot{\varphi}\varepsilon_\varphi + \dot{z}\varepsilon_z\right)\right]$$

$$(2)\quad \ddot{z} = \frac{qc^2}{E}\left[\varepsilon_z + r\dot{\varphi}B_r - rB_\varphi - \frac{\dot{z}}{c^2}\left(\dot{r}\varepsilon_r + r\dot{\varphi}\varepsilon_\varphi + \dot{z}\varepsilon_z\right)\right]$$

$$(3)\quad \ddot{\varphi} = -\frac{2\dot{r}\dot{\varphi}}{r} + \frac{qc^2}{rE}\left[\varepsilon_\varphi + \dot{r}B_z - \dot{z}B_r - \frac{r\dot{\varphi}}{c^2}\left(\dot{r}\varepsilon_r + r\dot{\varphi}\varepsilon_\varphi + \dot{z}\varepsilon_z\right)\right]$$

where: (r, φ, z) – coordinates of particle; (B_r, B_φ, B_z), $(\varepsilon_r, \varepsilon_\varphi, \varepsilon_z)$ – components of magnetic and electric fields; q – particle charge; c – speed of light; E – total energy of particle, the point above the coordinates indicates differentiation with respect to time. The method of Runge–Kutta of 4-order is used for integrating the equations. All calculations are fulfilled in the regime of double precision.

Cyclotron magnetic field is introduced into the program in the form of the table average value, amplitudes and phases of Fourier's harmonic in the median plane. Magnetic field created by beam current is not considered in the code. Electric fields are represented as sum of the accelerating high-frequency field and the space charge field:

$$(4)\quad \varepsilon_{r,\varphi,z} = \varepsilon^{\mathrm{RF}}_{\varphi,z} + \varepsilon^{\mathrm{SC}}_{r,\varphi,z}.$$

At each step of integration a particle gets, or loses energy in accordance with the sign of the expression:

$$(5)\quad \Delta w = q(\dot{r}\varepsilon_r + r\dot{\varphi}\varepsilon_\varphi + \dot{z}\varepsilon_z)\Delta t$$

where: Δt – step of integration.

Accelerating field is described by the expression:

$$(6)\quad \varepsilon^{\mathrm{RF}}_{\varphi,z} = \varepsilon^{\max}_{\varphi,z}\cos\left(2\pi\int_0^t (t)dt + \psi\right)$$

where: $f(t)$ – frequency program of synchrocyclotron (for the case of cyclotron this is constant); ψ – starting phase of particle. For calculating the amplitudes $\varepsilon_\varphi^{\max}$, $\varepsilon_z^{\max}$ the analytical description [5] is used:

$$(7)\quad \varepsilon^{\max}_\varphi = \frac{U}{S\sqrt{2\pi}}\exp\left(-0.5\cdot(y/S)^2\right)$$

$$(8)\quad \varepsilon^{\max}_\varphi = \frac{yz}{S^2}\varepsilon^{\max}_\varphi\left\{1 + \frac{1}{6}\left(\frac{z}{S}\right)^2\left[\left(\frac{y}{S}\right)^2 - 3\right]\right\}$$

where: $S = 0.2\,H + 0.4\,W$ (see Fig. 1), U – accelerating voltage.

Calculation of the beam electric field

Two methods were realised for calculating the beam space charge field: the method of pairwise interactions (particle-to-particle, PTP) and the method of particle in cell (particle-in-cell, PIC). In both methods the calculation of field is performed in the coordinate system, which moves together with the bunch. For the passage into the laboratory frame, in which the equations of motion are integrated, formulas from [7] are used.

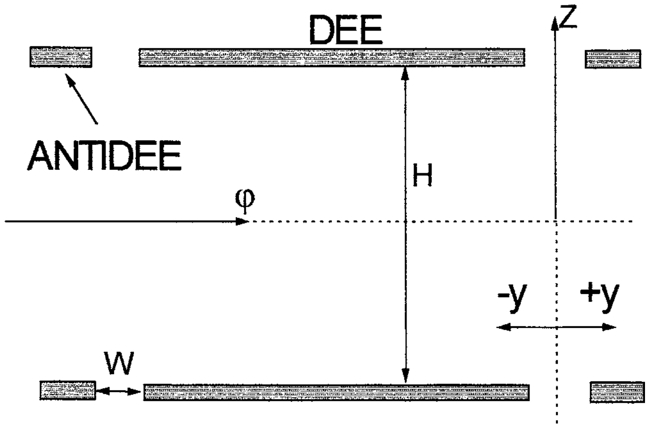

Fig. 1. Dee cross section geometry.

In the PTP method for a bunch, which consists of N macroparticles, the electric field acting on i-th particle is obtained via the summation of electric fields of all particles according to the following formulas:

$$(9)\quad \varepsilon(i)^{\mathrm{SC}}_r = \frac{q}{4\pi\varepsilon_0}\left[\cos\varphi_i\sum_{k=1}^{k=N}(x_i - x_k)/d^3_{ik} + \sin\varphi_i\sum_{k=1}^{k=N}(y_i - y_k)/d^3_{ik}\right]$$

$$(10)\quad \varepsilon(i)^{\mathrm{SC}}_\varphi = \frac{q}{4\pi\varepsilon_0}\left[\cos\varphi_i\sum_{k=1}^{k=N}(y_i - y_k)/d^3_{ik} - \sin\varphi_i\sum_{k=1}^{k=N}(x_i - x_k)/d^3_{ik}\right]$$

$$(11)\quad \varepsilon(i)^{\mathrm{SC}}_z = \frac{q}{4\pi\varepsilon_0}\sum_{k=1}^{k=N}(z_i - z_k)/d^3_{ik}$$

where: d_{ik} – distance between the i-th and k-th particles; (x, y, z) – Cartesian coordinates of particles; q – charge of macroparticle; $\varepsilon_0 = 8.85 \times 10^{-12}$ F/m. The given formulas are used if the distance between centres of two macroparticles exceeds their root-mean-square diameter. Otherwise, the formulas which describe electric field inside the uniform charged sphere are used.

The bases of the PIC method examplified on a two-dimensional model are presented in [8]. Our scheme of the three-dimensional computation of beam electric field appears as follows. The distribution of the space charge density in the region having the form of parallelepiped with the dimensions $a_x a_y a_z$ is examined at every step of integration of particle equations of motion. The parallelepiped is divided into the cells, whose vertexes form the nodes of three-dimensional calculation grid. Grid size in all dimensions changes and follows the dimensions of bunch. This approach makes it possible to preserve the number of particles in one cell as approximately constant in the process of computing the field of bunch. The space charge field is obtained as a result of solving Poisson's equation in the three-dimensional Cartesian coordinates:

$$(12)\quad \frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2} + \frac{\partial^2 U}{\partial z^2} = -\frac{\rho(x, y, z)}{\varepsilon_0}$$

with zero boundary conditions for the potential on the boundaries of the grid:

$$(13)\quad U(0,y,z) = U(a_x,y,z) = U(x,0,z) = U(x,a_y,z) = U(x,y,0) = U(x,y,a_z) = 0.$$

Poisson's equation is written in the finite differences:

$$(14)\quad \frac{U_{i+1,j,k}-2U_{i,j,k}+U_{i-1,j,k}}{h_x^2}+\frac{U_{i,j+1,k}-2U_{i,j,k}+U_{i,j-1,k}}{h_y^2}+\frac{U_{i,j,k+1}-2U_{i,j,k}+U_{i,j,k-1}}{h_z^2}=-\frac{\rho_{i,j,k}}{\varepsilon_0}.$$

The charge of each particle with the coordinates $\{x_n,y_n,z_n\}$ is distributed among the nearest eight grid points inversely proportional to a distance from the particle to each node:

$$(15)\quad \rho_{i,j,k}=q\sum_{n=1}^{N}\left(1-\frac{|x_n-x_i|}{h_x}\right)\left(1-\frac{|y_n-y_j|}{h_y}\right)\left(1-\frac{|z_n-x_k|}{h_z}\right)$$

$$(16)\quad h_x=\frac{a_x}{N_x},\ h_y=\frac{a_y}{N_y},\ h_z=\frac{a_z}{N_z}$$

where N_x, N_y, N_z – are numbers of partitions of grid in x, y and z directions. These numbers are multiple to the degree of number 2. Found this way the charge density and potential are represented in the form of Fourier series:

$$(17)\quad \rho_{m,n,p}=\sum_{i=1}^{N_x}\sum_{j=1}^{N_y}\sum_{k=1}^{N_z}\tilde{\rho}_{i,j,k}\sin\left(\frac{\pi mi}{N_x}\right)\sin\left(\frac{\pi nj}{N_y}\right)\sin\left(\frac{\pi pk}{N_z}\right)$$

$$(18)\quad U_{m,n,p}=\sum_{i=1}^{N_x}\sum_{j=1}^{N_y}\sum_{k=1}^{N_z}\tilde{U}_{i,j,k}\sin\left(\frac{\pi mi}{N_x}\right)\sin\left(\frac{\pi nj}{N_y}\right)\sin\left(\frac{\pi pk}{N_z}\right).$$

With this description the Fourier's coefficients of the charge density $\tilde{\rho}_{i,j,k}$, are connected with Fourier's coefficients of potential $\tilde{U}_{i,j,k}$ by the simple algebraic correlation:

$$(19)\quad \tilde{U}_{i,j,k}=\frac{\tilde{\rho}_{i,j,k}}{\dfrac{\sin^2\left(\dfrac{\pi i}{N_x}\right)}{h_x^2}+\dfrac{\sin^2\left(\dfrac{\pi j}{N_y}\right)}{h_y^2}+\dfrac{\sin^2\left(\dfrac{\pi k}{N_z}\right)}{h_z^2}}.$$

To compute the coefficients $\tilde{\rho}_{i,j,k}$, we used the procedure [4] of fast Fourier analysis. After the determination of the Fourier's coefficients of the potential $\tilde{U}_{i,j,k}$, the values of their own potential of beam in the grid points are calculated with the aid of the fast Fourier's synthesis [4]. Field that acts on the particle is computed by the help of a linear interpolation of field in the grid nodes taking into account the location of particle.

Results of SCE simulation in the cyclotron

The cyclotron–injector has a magnetic structure which consists of four separated sectors and accelerating system with two Δ-electrodes. Some parameters of the cyclotron are given in Table 1. The simulation of particle dynamics was only done for the bunch accelerated during 5 revolutions, necessary to get the final energy of 5 MeV. The initial set of particles was obtained via the random sampling inside a 6-dimensional phase volume of the bunch. This volume was matched with the acceptance of cyclotron at the point of injection (middle of the sector magnet) taking into account SCE. The normal distribution of particle density over all coordinates of phase space was assumed. From 200 to 10,000 particles were used in the calculations. Time step of the integration of equations was equivalent to the particle azimuth displacement by ~0.5°.

Table 1. Some parameters of the cyclotron.

Type of accelerated particle		H^-
Initial energy	(MeV)	0.5
Final energy	(MeV)	5.0
Average magnetic field	(T)	0.43
Betatron frequencies ν_r, ν_z		1.1, 0.8–0.9
Radius of injection	(cm)	27.0
Radius of extraction	(cm)	75.0
Emittance on injection ε_r, ε_z	(π mm·mrad)	60.0, 30.0
Bunch phase width	(°RF)	20
Orbital frequency	(MHz)	6.7965
Harmonic number		8
Number of accelerating gaps		4
Accelerating voltage (increase with radius)	(kV)	160–300

In the PIC method of space charge calculation the 3-dimensional grid with the number of cells 32 × 32 × 32 was used. The root-mean-square dimensions of bunch in three directions were calculated at every step of integration. In order the calculated grid deliberately cover entire beam its physical dimensions composed $\pm 6\sigma_{x,y,z}$, where σ is standard deviation of the beam size.

Figure 2 shows how differ the final values of the root-mean-square (±2σ) emittances (including energy spread) of beam for the two methods depending on the number of macroparticles with the accelerated current 15 mA. (Graph points at the beginning of the curves corresponding to computation 200 macroparticles without SCE.) It follows

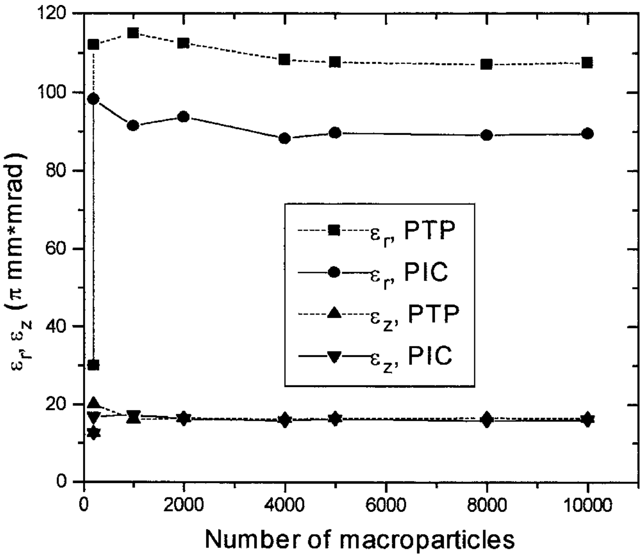

Fig. 2. Final values of the transverse emittances for two methods of SCE depending on the number of macroparticles.

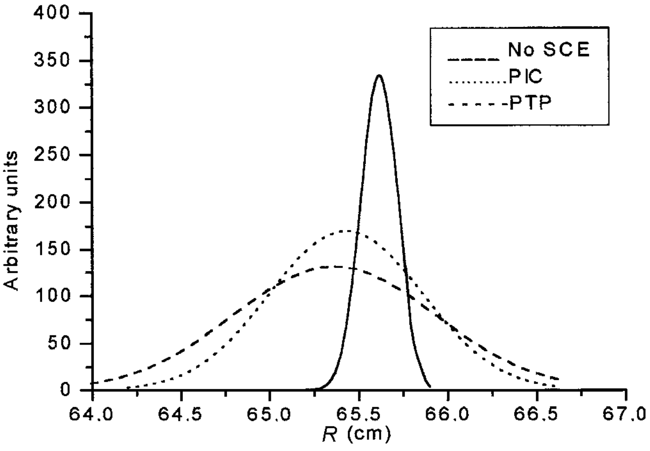

Fig. 3. Distribution of particle density across the bunch at final turn (I = 15 mA).

from Fig. 2 that the emittances of beam weakly depend on the number of macroparticles. It is observed, if the number of macroparticles is more than several thousand, then spectra of the values of electric field of beam at any chosen moment of acceleration will experience insignificant variation within 1–5% in spite of large change in the number of macroparticles. Similar results were obtained in [2].

There is a difference of ~20% between the values of the radial emittance, obtained with the aid of the PIC and PTP methods of computation. Axial emittances coincide in limits ±3%. We should explain the reason for the disagreement of the results on radial motion in further work. Distributions of particle density across the radial section of bunch at final turn are shown in Fig. 3 for different conditions of computation. Full radial size of the bunch is increased from 7 mm, when no space charge to ~25 mm under space charge influence.

Figures 4 and 5 illustrate the influence of SCE on the radial and axial dimensions of beam in the entire period of acceleration in case when the PIC method is used. The PTP method gives very similar results. It is evident that the space charge leads to a change of the dimensions of beam in both directions, but its influence on the radial motion is more substantial. The free radial zone between 4th and 5th revolutions, required for the effective beam extraction, is reduced from 70 mm in the absence SCE, to 45 mm and 30 mm, with 15 mA and 30 mA of beam current, accordingly. Calculations showed also that SCE led to an increase in the beam energy spread in the last orbit from ±2.2% to ±3.4% (current 15 mA).

Conclusions

Both methods of the calculation of space charge lead to close results on the electric field of beam and particle dynamics. The final values of the transverse emittances do not depend on the number of macroparticles (with the same simulated current), if the number of macroparticles is composed of several thousand. If matching of the form of injected beam on the axial phase plane is carried out, taking into account subsequent action of space charge, it is possible to avoid a noticeable increase in the axial size of beam. The radial separation of orbits on the last revolution in the cyclotron remains clear up to the beam current of 30 mA.

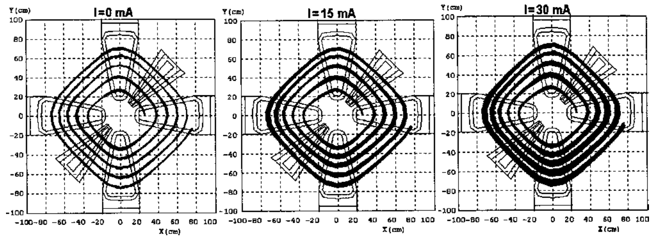

Fig. 4. Plan view on the orbits of 5000 particles at different intensity of the beam.

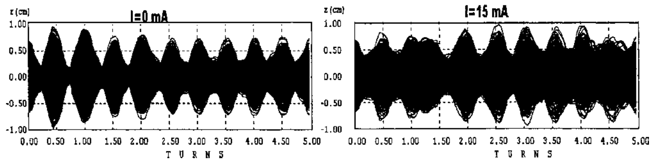

Fig. 5. Comparison of axial particle trajectories during the acceleration. To the left – there are no SCE, to the right – taking into account SCE (I = 15 mA).

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