Simulation of beam gas coulomb scattering in HALS*

YU Lu-Xin(于路新)[1)] GAO Wei-Wei(高巍巍)[2)] WANG Lin(王琳)[3)] LI Wei-Min(李为民)

NSRL, School of Nuclear Science and Technology,
University of Science and Technology of China, Hefei 230029, China

Abstract: In conventional research on beam gas coulomb scattering (BGCS), only the related beam lifetime using the analytical method is studied. In this paper, using the particle-in-cell Monte Carlo collisions (PIC-MCC) method, we not only simulated the beam lifetime but also explored the effect of BGCS on the beam distribution. In order to better estimate the effect on particle distribution, we study the ultra-low emittance electron beam. Here we choose the HeFei Advanced Light Source. By counting the lost particles in a certain time, the corresponding beam lifetime we simulated is 4.8482 h/13.8492 h in x/y, which is very close to the theoretic value (5.0555 h /13.7024 h in x/y). By counting the lost particles relative to the collided particles, the simulated value of the loss probability of collided particles is 1.3431e-04, which is also very close to the theoretical value (1.3824e-04). Besides, the simulation shows there is a tail in the transverse distribution due to the BGCS. The close match of the simulation with the theoretic value in beam lifetime and loss probability indicates our simulation is reliable.

Key words: beam gas coulomb scattering, elastic collision formula, beam lifetime, beam distribution

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1 Introduction

In an e-storage ring, there is always some residual gas near the beam orbit, no matter how efficient the vacuum condition is. The electrons will inevitably collide with it. The interaction between the electrons and residual gas is quite complex. There are mainly three mechanisms: the coulomb scattering, bremsstrahlung scattering, and the inelastic scattering with the outer-shell electron. These collisions will cause the change of the beam electron motion state; if the change is large enough, the corresponding electron will be lost. In the three types of beam gas interaction, the most common and basic is the coulomb scattering on the nucleus which is called beam gas coulomb scattering (BGCS). This forms the topic of our study in this paper [1].

Conventionally, the analytical method is the most common way to study BGCS [2, 3], and the analysis is always limited to obtain the calculation formula of the beam lifetime. In recent years minority or individual researches try to simulate beam lifetime using the MC method [4].

But does the beam gas scattering just affect the beam lifetime? What about the particle distribution? We explore the process of particle loss. First the momentum of the collided particle is changed due to the scattering. Then along with the beam transport, the position of the particle is changed. At last, the particle will be lost if it exceeds the limited conditions. From this process, it can be seen that the beam lifetime is also based on the change of particle distribution. Unfortunately, there is no research on the BGCS influence on particle distribution.

In this paper, using the particle-in-cell Monte Carlo collisions (PIC-MCC) method and choosing an appropriate cross section and scattering angle, we not only simulated the beam lifetime but also explored the effect of BGCS on the beam distribution. Moreover, previous studies on BGCS just gave a kick to transverse oscillation. In order to get the post-momentum of the particles more accurately, we deal with the collision process in a laboratory coordinate system.

This paper is organized as follows: In Section 2 the basic theory is given. In Section 3 the simulation technique is described. The results of the simulation are compared with the theoretic study in Section 4, and Section 5 is devoted to a discussion and conclusion.

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1) E-mail: yuluxin@mail.ustc.edu.cn

2) E-mail: gaomqr@mail.ustc.edu.cn

3) E-mail: wanglin@ustc.edu.cn

2 Basic theory of the simulation

2.1 The PIC-MCC method [5, 6]

The PIC-MCC method is a numerical technique in many-charged-particles simulation that has been widely used for decades. It attempts to balance the PIC and MCC. With the PIC-MCC method to track the motion of massive particles, all the micro information of the particle system is included. Any information, whether microcosmic or macroscopic, in principle, can be obtained.

Using the PIC-MCC to describe the collision of particles, the collision probability during one time-step Δt can be obtained by the following expression [6]:

$$p(t)=1-\exp(-\sigma\rho\nu\Delta t), \tag{1}$$

where σ is the collision cross section, ρ is the volume density of target particles, ν is the relative velocity of collided particles.

We generated a uniformly distributed random number $R_i\in[0\ 1]$, and by comparing the $p(t)$ with R_i, determined if the particle can collide. If R_i was less than $p(t)$, the particle suffered a collision, then it was processed by the MCC method. If R_i was larger than $p(t)$, the particle did not collide, then it was processed by the PIC method.

2.2 The derivation of collision formulas

By transferring the collision into the centre of mass reference frame (CM), Vincenti and Kruger give the formulas of collision between two non-relativistic particles [7]. The main points are shown in Fig. 1.

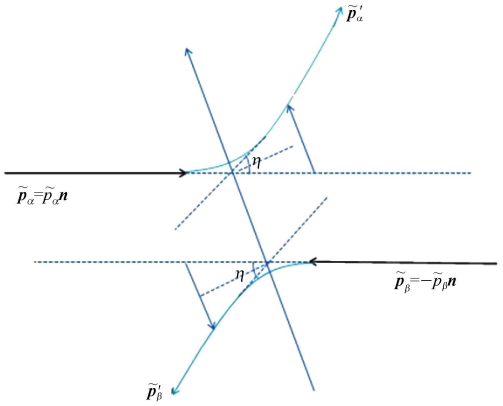

Fig. 1. The trajectories of two particles during a collision in the CM frame.

In Fig. 1, the initial momenta ($\boldsymbol{p}_\alpha$, $\boldsymbol{p}_\beta$) of the two collided particles (α, β) are equal and opposite. Furthermore, the force on each of the two particles is equal in magnitude but opposite in direction. As a result the final momenta deflecting at an angle η are also equal and opposite. With (p'_α, p'_β) these results conservation of total momentum and energy have been satisfied, and the final momenta can be written in terms of the initial momenta and η. The η is defined in the CM frame.

But it will be more complex to obtain the post-momenta of relativistic particles, which need twice Lorenz transformation [8]. In our simulation, we just need the electron's post-momentum. Combining the above points, we deal with the collision in a laboratory coordinate system. Below is the description.

For electron-atom elastic collision, the atom is considered to have a so large mass relative to the electron that the electron only scatters in angle χ with no loss of energy [5]. So the electron's trajectory in a laboratory coordinate system can be described as shown in Fig. 2.

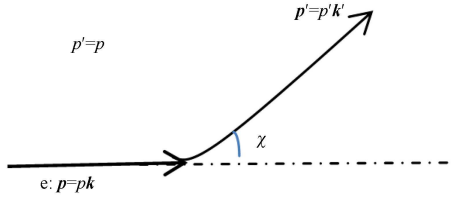

Fig. 2. The electron's deflection in a laboratory coordinate system.

Where, $\boldsymbol{k}$ is the unit vector of $\boldsymbol{p}$, while $\boldsymbol{k}'$ is the unit vector of $\boldsymbol{p}'$, so the electron's collision process can be described as $|\boldsymbol{p}|=|\boldsymbol{p}'|$ with the direction changed from $\boldsymbol{k}$ to $\boldsymbol{k}'$.

Since the $p'=p$, if the component of $\boldsymbol{k}'$ is known, $\boldsymbol{p}'$ will be easy to get. Now what we should do is find the relationship between $\boldsymbol{k}'$ and $\boldsymbol{k}$. Fig. 3 shows the relationship between $\boldsymbol{k}'$ and k.

On the left of Fig. 3, the components of $\boldsymbol{k}$ in (x, y, s) can be obtained by equation (2) [7].

$$\begin{pmatrix}\cos\theta\cos\varphi & \cos\theta\sin\varphi & -\sin\varphi\\ -\sin\varphi & \cos\varphi & 0\\ \sin\theta\cos\varphi & \sin\theta\sin\varphi & \cos\theta\end{pmatrix}\begin{pmatrix}k_x\\k_y\\k_s\end{pmatrix}$$
$$=\begin{pmatrix}0\\0\\k\end{pmatrix}\Leftrightarrow\begin{pmatrix}k_x\\k_y\\k_s\end{pmatrix}=\begin{pmatrix}k\sin\theta\cos\phi\\k\sin\theta\sin\phi\\k\cos\theta\end{pmatrix} \tag{2}$$

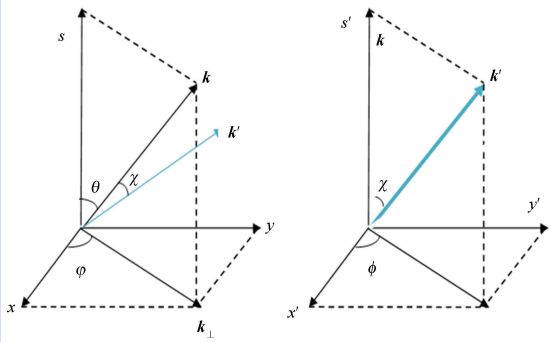

Fig. 3. The vector diagram of $\boldsymbol{k}$ and $\boldsymbol{k}'$.

Similarly, on the right of Fig. 3, there is a relationship for $\boldsymbol{k}'$ in (x', y', s').

$$\begin{pmatrix} \cos\chi\cos\phi & \cos\chi\sin\phi & -\sin\phi \\ -\sin\phi & \cos\phi & 0 \\ \sin\chi\cos\phi & \sin\chi\sin\phi & \cos\chi \end{pmatrix} \begin{pmatrix} k'_{x'} \\ k'_{y'} \\ k'_{s'} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ k' \end{pmatrix} \Leftrightarrow \begin{pmatrix} k'_{x'} \\ k'_{y'} \\ k'_{s'} \end{pmatrix} = \begin{pmatrix} k'\sin\chi\cos\phi \\ k'\sin\chi\sin\phi \\ k'\cos\chi \end{pmatrix}. \tag{3}$$

Where the angle ϕ takes on values from 0 to 2π.

So $\boldsymbol{k}'$ in (x, y, s) has the following relationship.

$$\begin{pmatrix} \cos\theta\cos\varphi & \cos\theta\sin\varphi & -\sin\varphi \\ -\sin\varphi & \cos\varphi & 0 \\ \sin\theta\cos\varphi & \sin\theta\sin\varphi & \cos\theta \end{pmatrix} \begin{pmatrix} k'_{x'} \\ k'_{y'} \\ k'_{s'} \end{pmatrix} = \begin{pmatrix} k'\sin\chi\cos\phi \\ k'\sin\chi\sin\phi \\ k'\cos\chi \end{pmatrix}. \tag{4}$$

It can be driven

$$\begin{Bmatrix} k'_x \\ k'_y \\ k'_s \end{Bmatrix} = \begin{Bmatrix} k'\cos\chi\cos\varphi\sin\theta+k'\sin\chi\cos\theta\cos\varphi\cos\phi-k'\sin\chi\sin\varphi\sin\phi \\ k'\cos\chi\sin\varphi\sin\theta+k'\sin\chi\cos\theta\sin\varphi\cos\phi+k'\sin\chi\cos\varphi\sin\phi \\ k'\cos\theta\cos\chi-k'\sin\chi\cos\phi\sin\theta \end{Bmatrix}. \tag{5}$$

Taking $k'=k=1$ and Eq. (2) into Eq. (5):

$$\begin{Bmatrix} k'_x \\ k'_y \\ k'_s \end{Bmatrix} = \begin{Bmatrix} k_x\cos\chi+k_xk_s/k_\perp\sin\chi\cos\phi-k_y/k_\perp\sin\chi\sin\phi \\ k_y\cos\chi+k_yk_s/k_\perp\sin\chi\cos\phi-k_x/k_\perp\sin\chi\sin\phi \\ k_s\cos\chi-k_\perp\sin\chi\sin\phi \end{Bmatrix}. \tag{6}$$

Taking $k_x=p_x/p$, $k_y=p_y/p$, $k_s=p_s/p$, $k_\perp=p_\perp/p$ into Eq. (6); then the post-collision momentum in a laboratory coordinate system for an elastic collision is given by

$$\boldsymbol{p}'=\boldsymbol{p}'\boldsymbol{k}'=\boldsymbol{p}\cos\chi+\boldsymbol{h}\sin\chi, \tag{7}$$

where $\boldsymbol{h}=(h_x, h_y, h_s)$ with

$$\begin{aligned} h_x &= (p_xp_s\cos\phi-p_yp\sin\phi)/p_\perp \\ h_y &= (p_yp_s\cos\phi-p_xp\sin\phi)/p_\perp \\ h_s &= -p_\perp\cos\phi. \end{aligned} \tag{8}$$

where ϕ is uniformly distributed in [0, 2π]. χ is an angle defined in a laboratory coordinate system.

It should be clearly noted that although Eq. (7) is obtained under a laboratory coordinate system, though the collision is instantaneous, it also applies to the Frenet-Serret coordinate system.

With the collision formulas, we will investigate the beam lifetime and the particle distribution's change caused by the coulomb scattering with the residual gas atoms.

3 Simulation method

3.1 The description of the simulation method [4]

The simulation is based on the macro-particle method. The macro-particles transfer through the ring and encounter coulomb scattering with residue gas atoms simultaneously.

The initial 6-D coordinates of n macro-particles are given randomly with specified variances. Each macro-particle (i) has a particle number (N_i). ΣN_i is the total number of particles in a bunch.

We set one fixed interaction point (IP) in the ring, and used one turn transfer map to transmit the particle. We define p as the probability that an electron scattering collides with the gas nucleus in one turn. So the probability that each macro-particle undergoes a random process is N_ip.

For each macro-particle, a random number $R\in\infty[0,1]$ is chosen each turn, if $R<N_ip$, we separate one electron from the i-th macro-particle as a new macro-particle. The new macro-particle has the same coordinates to the parental macro-particle.

During the collision, the (p_x, p_y, p_s) of the new macro-particle is changed, while the (x, y, s) is considered the same as before. The new macro-particle will not undergo the BGCS again, it just propagates in the ring.

As a result of the specific aperture, this process will lead to the loss of particles. Then the beam lifetime of the beam will be estimated in the simulation by counting the number of the particles extending beyond the specific aperture.

3.2 The choice of cross section and scattering angle

In a previous simulation, only the scattering that would cause the particle loss is considered to obtain the beam lifetime. Whether the particle would be lost depends on the relationship of the scattering angle and the critical angle. The critical angle is the minimum angle which would cause particle loss. The electron loss cross section is used to calculate the loss probability. Now that

we are going to explore the effect of gas scattering on particle distribution, we should take into account all the scatterings. So we choose the appropriate cross section and scattering angle, rather than the particle loss section and critical scattering angle, to simulate the BGCS.

For the relativistic electrons collisions, the knowledge of the screening of the coulomb potential of the nuclei by the atomic electrons is important, since they are always scattered into a very small angle. The differential cross section that contains the shielding effect of the electron cloud can be determined by [9, 10].

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}=\frac{4Z^2}{a_h^2}\frac{\gamma^2}{\left[\left(\frac{4\pi}{\lambda_\mathrm{e}}\sin\frac{\chi}{2}\right)^2+\frac{1}{R^2}\right]^2}, \tag{9}$$

where Ω is the solid angle, χ the scattering angle, Z the atomic number, λ_e the wave-length of the electron, γ the Lorentz factor and the radius of atom $R=a_h*Z^{-1/3}$. a_h is the Bohr's radius of the atoms.

By integrating Eq. (9) over the whole Ω, we can obtain the total cross section

$$\sigma=\left(\frac{4Z\gamma}{a_h}\right)^2\left(\frac{\lambda_\mathrm{e}}{4\pi}\right)^4\left(\frac{1}{2\varepsilon}-\frac{1}{2+2\varepsilon}\right). \tag{10}$$

With $\varepsilon=(\lambda_\mathrm{e}/4\pi R)^2$ is the shielding parameter.

During the simulation, a random number generator is used at each turn to decide whether the scattering occurs. If yes, the scattering angle is defined according to the following formula [8]:

$$\chi=\frac{\pi}{2}-\arcsin\left[1-\frac{2R_1}{1-(R_1-1)(4\pi R/\lambda_\mathrm{e})^2}\right]. \tag{11}$$

where R_1 is uniformly distributed from 0 to 1.

The distribution of the scattering angle under different energy levels is shown in Fig. 4 and Fig. 5. It can be seen that the higher energy the electron is, the smaller angle the electron will be scattered at. Conversely, the scattering angle tends to be uniform from 0 to pi for nonrelativistic electrons. This is consistent with theoretical analysis, which also shows the formula is reasonable and reliable. For the HALS, the energy of the electron is 1.8 GeV, and the probability that the scattering angle is smaller than 2.5808e-5 rad is 98%.

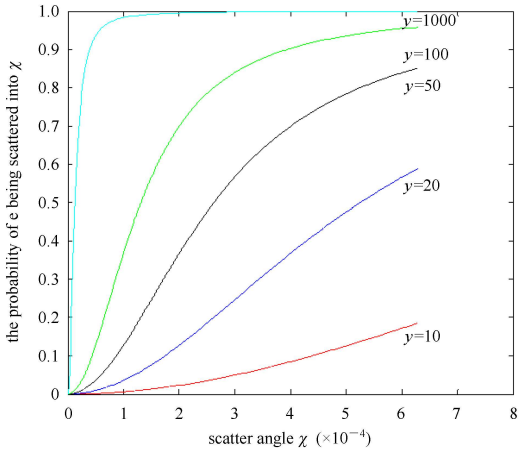

Fig. 4. (color online) The collision probability of the electron with different energy levels being scattered into an angle χ.

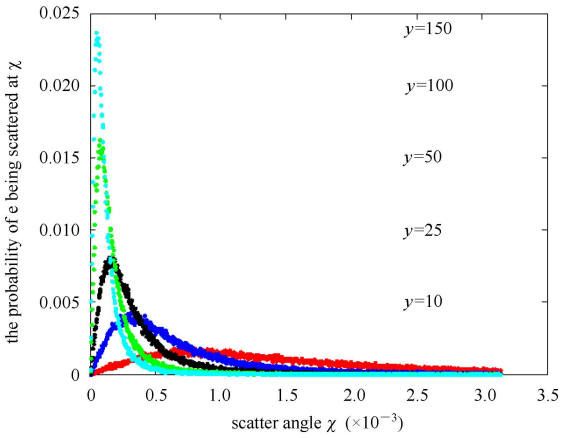

Fig. 5. (color online) The distribution of the scattering angle under different energy levels

4 Simulation results

In the simulation, because a secondary collision of the newly generated macro-particles hardly occurs, we assume the new micro-particles will not undergo the BGCS again. For this reason, the number of initial micro-particles should not be less than the number of collided electrons in one turn. For HALS, about 7810 ($n_e p$) electron collisions occur in a turn, we set 8e5 (about 100 times the collided particles) initial macro-particles. The total number of particles is 1e10, so each initial macro-particle contains 12500 electrons.

Table 1. Simulation parameters of HALS.

parameter	description	value
E	beam energy	1.8 GeV
C	circumference	486 m
n_e	particles in bunch	10^{10}
H	harmonic number	810
β_IP	twiss parameter beta	9.1307/3.4663
α_IP	twiss parameter alpha	−1.83e-3/5.6151e-5
γ_IP	twiss parameter gamma	0.1095/0.2885
ε_x	Hor. emittance	62 pm·rad
ε_y	Ver. emittance	0.62 pm·rad
d	dynamics aperture	2.4/1.5 mm
P	N_2-equivalent gas pressure	1ntorr

The vacuum is expressed by N_2-equivalent gas pressure. In order to verify the program, it is supposed that

there is only N_2 in the ring. Each N_2 molecule has two atoms with atomic number 7. Table 1 shows the simulation parameters of HALS.

Moreover, in order to eliminate the MC fluctuation, we run the simulation five times, and take the statistical average.

4.1 The lifetime of a beam

Once a particle's amplitude exceeds an aperture, which is the dynamics aperture in this paper, this particle will be lost.

In the simulation, lost particles are counted each turn. Fig. 6 shows the number of lost particles growing with time.

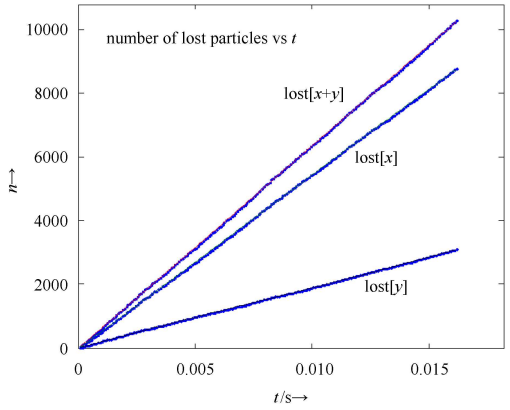

Fig. 6. The number of lost particles with time.

The simulation lifetime of a beam can be calculated by the following formula.

$$n=n_{\rm e}{\rm e}^{-t/\tau}. \tag{12}$$

Where n is the number of total particles after time t, while $n_{\rm e}$ is the number of initial particles. With the date in Fig. 6, the simulation beam lifetime is 5.1078 h/14.5507 h in x/y. Note that the lifetime in our simulation is the lifetime at IP.

Now, what we have to do is to verify whether this simulation result is reasonable. The beam coulomb lifetime related to the vacuum can be obtained as below [11].

$$\frac{1}{\tau_{{\rm elastic},u}[s]}=\frac{2\pi r_{\rm e}^2 c}{K\gamma^2}\frac{\beta_u}{A_u T[^0K]}\sum_{{\rm atom},j}\left(Z_j^2\sum_{{\rm gas},i}\alpha_{ij}P_i[{\rm Pa}]\right). \tag{13}$$

With u presenting x or y. Taking $\beta_u=\beta_{\rm IP}$, $A_u=d_u^2/\beta_{\rm IP}$, $\beta_{{\rm IP},\mu}$ then the corresponding lifetime at IP is 5.0555 h/13.7024 h in x/y.

It can be seen the simulation lifetime (4.8482 h/13.8492 h) is very close to the theoretical value (5.0555 h/13.7024 h).

On the other hand, the critical scattering angle can be computed by the below [1].

$$\theta_{cx,y}=d_{x,y}/\beta_{x,y}. \tag{14}$$

Define $\sigma_{\rm loss}$ as the beam loss cross section. $\sigma_{\rm loss}$ equals the integration of Eq. (9) from $\theta_{\rm c}$ to π.

Taking the geometric mean of $\theta_{\rm c}$ in x and y, we have $\theta_{\rm c}$=3.3726e-04rad, then $\sigma_{\rm loss}$=3.4710e-27 m^2. With $\sigma_{\rm loss}/\sigma$, the theoretical loss probability of collided particles is 1.3824e-04.

In the simulation, take 10000 turns as an example, the number of electrons that collided with the gas nucleus is 77799091, the number of lost electrons is 10449, so the simulation value of the loss probability of the collided particles is 13.431e-04, which is very close to the theoretical value (1.3824e-04).

4.2 The distribution of particles

In Fig. 7, the red dots represent the initial distribution of particles, while the blue dots represent the particle distribution after 10000 turns. Visually, the particles have a diffusion in both x and y due to the beam gas coulomb scattering. One thing is for sure, the peripheral particles in the bunch after 10000 turns are mostly new macro-particles.

Figure 8 shows the horizontal and vertical statistical distributions of the particles in a bunch. The red dots represent the initial distribution, and the blue ones the distribution after tracking. It can be seen that there is a tail because of the beam gas scattering. The tail accounts for a little proportion of the total particles. In the horizontal direction, the proportion that ρ is less than -15 is 6.9994e-04. In the vertical direction, the proportion that ρ is less than -12 is 0.0029. The result shows the tail in y is larger than x. In our simulation, the bunch is much more concentrated in y, and there is no coupling

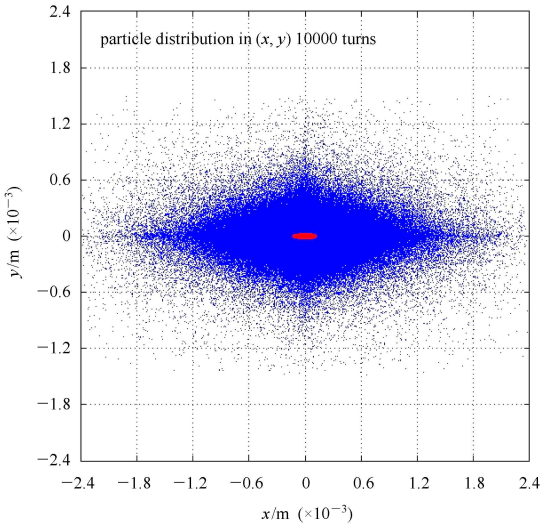

Fig. 7. The transverse distribution of particles.

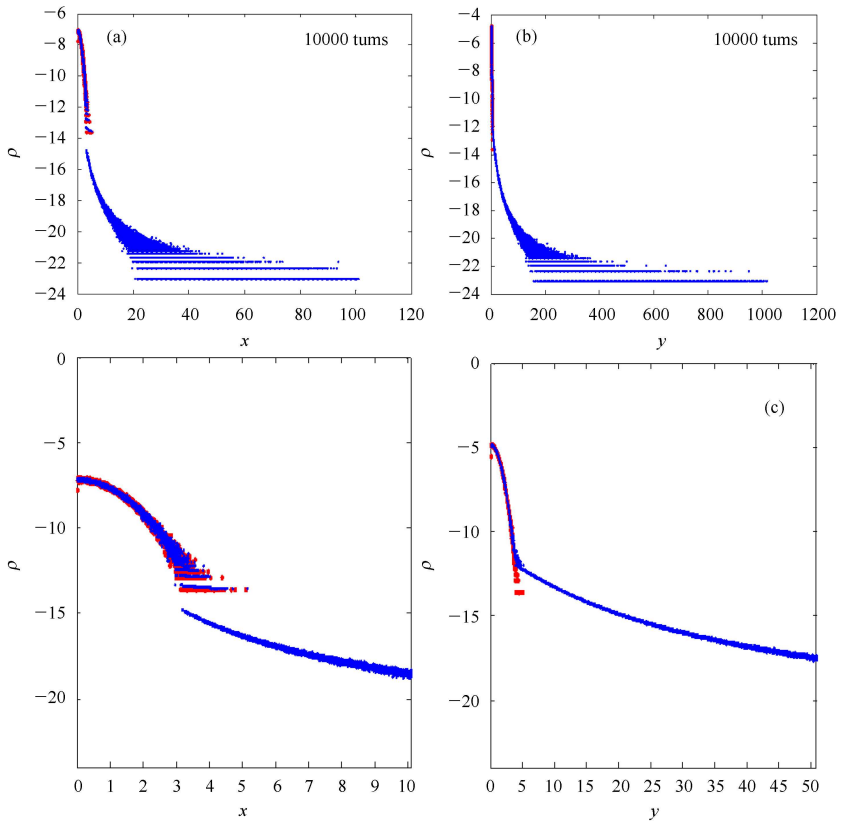

Fig. 8. The statistical distribution in transverse direction, the horizontal axis x/y is the distance normalized by the nominal horizontal/vertical beam size. The vertical axis represents the distributions in x/y using a logarithmic scale. The two pictures in (c) show the details in small distance.

in x and y. So we can conclude that the effect of BGCS on particle distribution depends on how much the bunch is diverging. This also means that the smaller the emittance is, the greater the effect.

5 Summary and outlook

In this paper, by deducing the collision formulas in a laboratory coordinate system and choosing an appropriate cross section and scattering angle, we simulate the effect of the BGCS in the ultra-low emittance electron storage ring using the PIC-MCC method. The results show that the BGCS not only relates to the beam lifetime but can also cause the transverse diffusion.

In future work, more random processes will be added to the simulation, such as more kinds of residual gases, inelastic scattering with residual gas, IBS, synchrotron radiation, etc. On the other hand, we are going to realize program parallelization to improve computational efficiency.

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