Theory of collision algorithms for gases and plasmas based on the Boltzmann equation and the Landau-Fokker-Planck equation

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A time-explicit formula that describes the time evolution of velocity distribution functions of gases and plasmas is derived from the Boltzmann equation. The formula can be used to construct collision simulation algorithms. Specialization of the formula to the case of the Coulomb interaction shows that the previous method [K. Nanbu, Phys. Rev. E **55**, 4642 (1997)] for a Coulomb collision simulation is a solution method of the Landau-Fokker-Planck equation in the limit of a small time step. Also, a collision simulation algorithm for multicomponent plasmas is proposed based on the time-explicit formula derived.

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I. INTRODUCTION

It is well known that there are very efficient schemes for the Monte Carlo simulation of collisional processes in rarefied gases with short-range intermolecular forces. Bird [1] developed the particle simulation method (DSMC) for rarefied gases by using the fundamental properties of gases such as the mean free path and the collision frequency. Although the method reflects many of the ideas and concepts employed in the derivation of the Boltzmann equation, it was regarded as a method for numerical experiments. After Bird's work, one of the present authors [2] derived a particle simulation method from the Bolzmann equation and clarified the theoretical background of Bird's method [3]. A comprehensive review of rigorous mathematical results on simulation methods for the Boltzmann equation can be found in the book of Cercignani, Illner, and Pulvirenti [4]. One can also mention many alternative numerical methods. For brevity, we refer only to two recently developed methods; one based on the fast Fourier transform [5] and the other based on Wild's sums [6]. Both methods are very interesting from a theoretical point of view. However, the practical computational efficiency in the case when the methods are applied to spatially inhomogeneous problems still appears to be much lower than the efficiency of the Bird-type schemes. Just for this reason, we here restrict our consideration to *traditional* Monte Carlo methods used in kinetic theory.

It is still unclear how to generalize the above methods to the case of long-range forces, in particular, to the Coulomb interaction. In this paper, the long-range forces are defined as the particle interaction for which the total collision cross section diverges within the framework of classical mechanics. We consider the Boltzmann equation for long-range forces and the Landau-Fokker-Planck equation from a unified point of view. Numerical methods based on a finite difference form of the latter equation were studied long ago (see, for example, Refs. [7] and [8]). It is very difficult, however, to apply such methods to spatially inhomogeneous problems. The same is true for methods based on the Langevin equation since the computational task increases roughly in proportion to the square of the number of simulated particles [9].

On the other hand, many articles have been published on methods of simulating Coulomb collisions on the basis of intuitive physical considerations. Some authors of these works attempted to show the consistency of their method with the Fokker-Planck equation. We cannot state, however, that these methods are derived from the Fokker-Planck equation. A representative selection of the published papers are referred to here. Takizuka and Abé [10] proposed a binary collision model that mimics the Fokker-Planck operator with the Landau form. Wang *et al.* [11] improved Takizuka and Abé's method, clarifying the relation between the proposed collision operator and the Fokker-Planck operator of the Landau form. Jones *et al.* [12] presented a method to calculate the force acting on a particle from grid quantities in the particle-in-cell codes. Their method was improved by Manheimer, Lampe, and Joyce [13] who introduced a weaker condition for the velocity distribution function.

In Coulomb collisions, small-angle collisions are much more important than collisions resulting in large velocity changes. It is this idea that Rosenbluth, MacDonald, and Judd [14] used to derive the Fokker-Planck equation from the Boltzmann equation. However, simulating small-angle collisions one by one is computationally inefficient. Cranfill, Brackbill, and Goldman [15] used the idea of grouping many small-angle collisions and succeeded in using a larger time step. One of the present authors [16,17] proposed a quite different formulation on a cumulative property of Coulomb collisions; the nature of his formulation yields a drastic decrease in computational effort in the particle simulation of Coulomb collisions. However, the unique simulation method [16] was proposed on the basis of physical considerations, without the use of any kinetic equation. Which equation does this method really solve? This is one of the questions we will attempt to answer. The aim of the present paper is to present a unified treatment of rarefied gases with long-range forces and plasmas on the basis of classical kinetic equations and to construct an efficient Monte Carlo collision algorithm for solving the kinetic equations. We should stress that some ideas of Ref. [16] were a starting point for the present paper.

The numerical schemes for kinetic equations are usually based on the splitting algorithm, namely, the collision process is treated separately from the motion of particles with-

out collisions. The problem of the collision process is to solve a spatially homogeneous kinetic equation. Given our goals, it is therefore sufficient to consider only the spatially homogeneous case.

The paper is organized as follows. In Sec. II we discuss the problem in detail. Then we introduce an important approximation to the Boltzmann equations for a simple gas (Sec. III) and mixtures (Sec. IV). The limiting case of small-angle scattering (the Landau-Fokker-Planck equation [18,19]) is considered in Sec. V, where a time-explicit kinetic equation for multicomponent plasmas is derived. This equation having first order accuracy in time step is similar in its Monte Carlo realization to the one used in Ref. [16]. Some simplified schemes are constructed in Sec. VI, where we also show that the scheme of Ref. [16] is really a method of solving the Landau-Fokker-Planck equation and that this scheme can be significantly simplified. In Sec. VII we derive a collision algorithm for mixtures using the formulation in Sec. V. A weight alogrithm is described in Sec. VIII, which is useful in simulating multicharged plasmas.

II. STATEMENT OF THE PROBLEM

Let $f(\mathbf{v},t)$ be a distribution function satisfying the spatially homogeneous Boltzmann equation:

$$\frac{\partial f}{\partial t}=\int_{R^3\times S^2} d\mathbf{w}d\mathbf{n}g\left(u,\frac{\mathbf{u}\cdot\mathbf{n}}{u}\right)[f(\mathbf{v}')f(\mathbf{w}')-f(\mathbf{v})f(\mathbf{w})], \tag{1}$$

where $\mathbf{v}$ is the particle velocity, t is the time, R^3 is 3-dimensional Euclidean space, S^2 is a unit sphere in R^3, $\mathbf{u}=\mathbf{v}-\mathbf{w}$, $u=|\mathbf{u}|$, $\mathbf{n}\in S^2$, i.e., $|\mathbf{n}|=1$, and

$$\mathbf{v}'=\frac{1}{2}(\mathbf{v}+\mathbf{w}+u\mathbf{n}),\quad \mathbf{w}'=\frac{1}{2}(\mathbf{v}+\mathbf{w}-u\mathbf{n}),$$
$$g(u,\cos\theta)=u\sigma(u,\theta),\quad (0\leqslant\theta\leqslant\pi). \tag{2}$$

Here $\cos\theta=\mathbf{u}\cdot\mathbf{n}/u$ and $\sigma(u,\theta)$ is the differential collision cross section at the scattering angle θ. The argument t is omitted in the distribution functions in Eq. (1).

We introduce also usual notations for integral cross sections

$$\sigma_{\rm tot}=2\pi\int_0^\pi d\theta\sigma(u,\theta)\sin\theta,$$
$$\sigma_{\rm tr}(u)=2\pi\int_0^\pi d\theta\sigma(u,\theta)\sin\theta(1-\cos\theta), \tag{3}$$

and note that $\sigma_{\rm tot}=\pi R_{\rm max}^2$ for intermolecular potentials with a finite radius $R_{\rm max}$ of action. For example, $R_{\rm max}=d$ for hard spheres of diameter d. We distinguish two alternative cases: (i) short-range potentials ($R_{\rm max}<\infty$) and (ii) long-range potentials ($R_{\rm max}=\infty$). In the first case we can rewrite Eq. (1) as

$$\frac{\partial f}{\partial t}=I^+-I^-,\quad I^-=f(\mathbf{v})\sigma_{\rm tot}\int_{R^3}d\mathbf{w}f(\mathbf{w})|\mathbf{v}-\mathbf{w}|, \tag{4}$$

and define a typical time interval τ_0 between two successive collisions (relaxation time) by

$$\frac{1}{\tau_0}=\sigma_{\rm tot}\left\langle\int_{R^3}d\mathbf{w}f(\mathbf{w})|\mathbf{v}-\mathbf{w}|\right\rangle, \tag{5}$$

where the average $\langle\cdots\rangle$ over $\mathbf{v}$ may be obtained by using the corresponding Maxwellian distribution. Equation (5) is, in a sense, a key point of any sort of DSMC method for Eq. (1). In DSMC methods we simulate binary collisions, keeping in mind that roughly speaking, the total number of collisions in a given time interval corresponds to Eq. (5). The methods obviously fail if $R_{\rm max}=\infty$ (long-range potentials) since $\tau_0=0$ in Eq. (5), and therefore the number of collisions is infinitely large in any given time interval.

On the other hand, the initial data problem for Eq. (1) is well posed for a certain class of potentials with $R_{\rm max}=\infty$; typical examples are $V(r)\propto 1/r^n (n>1)$ or $V(r)\propto e^{-\alpha r}/r$, α being a constant. In such cases, I^- in Eq. (4) loses its meaning although a typical relaxation time is still well defined, say, as

$$\frac{1}{\tau_1}=\left\langle\int_{R^3}d\mathbf{w}f(\mathbf{w})u\sigma_{\rm tr}(u)\right\rangle \tag{6}$$

with $u=|\mathbf{v}-\mathbf{w}|$. The physical reason for the solvability of Eq. (1) for long-range potentials is now very clear: An infinite number of small-angle collisions yields a finite contribution in the relaxation process. How can we simulate this process by DSMC methods? The simplest method is to introduce a radial cutoff of the potential $V(r)$ [or angular cutoff of the cross section $\sigma(u,\theta)$ at a small angle]. We thus obtain an approximate form of Eq. (4) with a *very large* $\sigma_{\rm tot}$ but we can use the standard DSMC method for Eq. (4). This approach is, however, rather inefficient since we need to choose the time step Δt which satisfies the condition $\Delta t<\tau_0=O(\sigma_{\rm tot}^{-1})$, whereas the true relaxation time τ_1 of Eq. (6) satisfies the inequality $\tau_1\gg\tau_0$. Another method to avoid the divergence of $\sigma_{\rm tot}$ is to regard $\sigma(u,\theta)$ as isotropic, i.e., independent of θ. This results in the variable hard-sphere model [20]. This model is very successful from the engineering point of view, but some arbitrariness remains when determining the constant in the model; one may use viscoscity, thermal conductivity, or self-diffusion coefficients.

All these considerations remain valid also for the Landau-Fokker-Planck equation for plasmas [18,19], which is simply an asymptotic form of the Boltzmann equation (1) for the Debye potential $V(r)\propto e^{-\alpha r}/r$ in the limit of $\alpha\to 0$.

We now ask: How can we construct an efficient DSMC method for long-range potentials? We attempt to construct a method satisfying the following minimal requirements.

(a) The computational task should be proportional to the number of simulated particles.

(b) The time step of order τ_1 of Eq. (6), not τ_0 of Eq. (5), should be allowed.

(c) The simulation method should be similar in realization to some of the existing DSMC methods for the Boltzmann equation.

(d) The method should be generalizable to the Landau-Fokker-Planck equation and to multicomponent gases and plasmas.

Of course, requirement (c) is not always necessary but it is very convenient in practical use. We now derive the

DSMC method satisfying all the above requirements. This is the main purpose of the present paper. First we explain a key idea in the following section.

III. FIRST ORDER EQUATION

We consider the Boltzmann equation (1) and rewrite it in the following form:

$$\frac{\partial f}{\partial t}=\int_{R^3} d\mathbf{w} J F(\mathbf{U},\mathbf{u}), \tag{7}$$

where $\mathbf{U}=(\mathbf{v}+\mathbf{w})/2$ denotes the center-of-mass velocity, $\mathbf{u}=\mathbf{v}-\mathbf{w}$ is the relative velocity, and

$$F(\mathbf{U},\mathbf{u})\equiv f\left(\mathbf{U}+\frac{\mathbf{u}}{2}\right) f\left(\mathbf{U}-\frac{\mathbf{u}}{2}\right)=f(\mathbf{v})f(\mathbf{w}). \tag{8}$$

The operator J acts only on the angular variable $\boldsymbol{\omega}=\mathbf{u}/u$ in such a way that

$$JF(\mathbf{U},u\boldsymbol{\omega})=\int_{S^2} d\mathbf{n} g(u,\boldsymbol{\omega}\cdot\mathbf{n})[F(\mathbf{U},u\mathbf{n})-F(\mathbf{U},u\boldsymbol{\omega})]. \tag{9}$$

We note that $\mathbf{U}$ and u play only the role of constant parameters in Eq. (9); one can define the action of the operator J on arbitrary function $\psi(\boldsymbol{\omega})$ by

$$J\psi(\boldsymbol{\omega})=\int_{S^2} d\mathbf{n} g(\boldsymbol{\omega}\cdot\mathbf{n})[\psi(\mathbf{n})-\psi(\boldsymbol{\omega})], \tag{10}$$

where we omitted the irrelevant argument u in the scattering indicatrix $g(u,\boldsymbol{\omega}\cdot\mathbf{n})$. Let us approximate the time derivative and the operator J in Eq. (7) by

$$\frac{\partial f(\mathbf{v},t)}{\partial t}\simeq\frac{f(\mathbf{v},t+\Delta t)-f(\mathbf{v},t)}{\Delta t},\quad J\simeq\frac{1}{\varepsilon}[\exp(\varepsilon J)-\hat{I}], \tag{11}$$

where $\hat{I}$ is the identity operator, and Δt and ε are assumed to be sufficiently small. Then the approximate equation reads as

$$f(\mathbf{v},t+\Delta t)-f(\mathbf{v},t)=\frac{\Delta t}{\varepsilon}\int_{R^3} d\mathbf{w}[\exp(\varepsilon J)-\hat{I}]F(\mathbf{U},\mathbf{u}). \tag{12}$$

Let us write

$$\varepsilon=\rho\Delta t,\quad \rho=\int_{R^3} d\mathbf{v} f(\mathbf{v},t)=\text{const}, \tag{13}$$

where ρ is the number density. Then we obtain the approximate equation

$$\begin{aligned} f(\mathbf{v},t+\Delta t)&=\frac{1}{\rho}\int_{R^3} d\mathbf{w}\exp(\rho\Delta t J)F(\mathbf{U},\mathbf{u})\\ &=\frac{1}{\rho}\int_{R^3} d\mathbf{w}\exp(\rho\Delta t J)f(\mathbf{v},t)f(\mathbf{w},t). \end{aligned} \tag{14}$$

This equation approximates the Boltzmann equation (7) within an accuracy of $O(\Delta t)$, so that it is not formally worse than any other first order (in Δt) approximation of Eq. (1). The reason why this equation is useful for long-range potentials is that the exponential operator $\exp(\tau J)$ has much better properties than the operator J itself. We shall see this below.

The operator J in Eq. (10) is well known in linear transport theory [21]. To construct the operator $\exp(\tau J)$, it is sufficient to solve the initial value problem for $\psi(\boldsymbol{\omega},\tau)$ as

$$\frac{\partial\psi}{\partial\tau}=J\psi,\quad \psi(\boldsymbol{\omega},0)=\psi_0(\boldsymbol{\omega}),\quad (\boldsymbol{\omega}\in S^2), \tag{15}$$

for arbitrary $\psi_0(\boldsymbol{\omega})$. We assume

$$\|\psi_0\|^2_{L_2(S^2)}=\int_{S^2} d\boldsymbol{\omega}\psi_0^2(\boldsymbol{\omega})<\infty,$$

then we have

$$\psi_0(\boldsymbol{\omega})=\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\psi_{lm}^{(0)}Y_{lm}(\boldsymbol{\omega}),$$

$$\psi_{lm}^{(0)}=\int_{S^2} d\boldsymbol{\omega}\psi_0(\boldsymbol{\omega})Y_{lm}^{*}(\boldsymbol{\omega}),$$

where $Y_{lm}(\boldsymbol{\omega})$ are the spherical function and $Y_{lm}^{*}(\boldsymbol{\omega})$ is its complex conjugate. Using the additional theorem for the spherical function, we can easily prove

$$JY_{lm}=-\lambda_l Y_{lm},\quad \lambda_l=2\pi\int_{-1}^{1} d\mu g(\mu)[1-P_l(\mu)]. \tag{16}$$

Therefore, the solution of Eq. (15) reads as

$$\psi(\boldsymbol{\omega},\tau)=\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\psi_{lm}^{(0)}\exp(-\lambda_l\tau)Y_{lm}(\boldsymbol{\omega}).$$

It is more convenient to express the solution in the following integral form:

$$\psi(\boldsymbol{\omega},\tau)=\exp(\tau J)\psi_0(\boldsymbol{\omega})=\int_{S^2} d\mathbf{n} G(\boldsymbol{\omega}\cdot\mathbf{n},\tau)\psi_0(\mathbf{n}), \tag{17}$$

where

$$G(\mu,\tau)=\sum_{l=0}^{\infty}\frac{2l+1}{4\pi}\exp(-\lambda_l\tau)P_l(\mu),\quad (-1\leqslant\mu\leqslant 1), \tag{18}$$

and $P_l(\mu)$ is the Legendre polynomial. We note that

$$\lim_{\tau\to 0+} G(\mu,\tau)=\frac{1}{2\pi}\delta(1-\mu). \tag{19}$$

A remark is here necessary: It follows from Eq. (16) that

$$\lim_{l\to\infty}\lambda_l=2\pi\int_{-1}^{1} d\mu g(\mu)=u\sigma_{\text{tot}}, \tag{20}$$

provided that $g(\mu)[\equiv g(u,\mu)]$ is given by Eq. (2). Therefore $g(u,\mu)$ is nonintegrable in $\mu\in(-1,1)$ for long-range

potentials, whereas the function $G(\mu,\tau)$, whose parameter τ is irrelevant, is even square integrable in this interval in typical cases. In this sense, it was mentioned above that $\exp(\tau J)$ has better mathematical properties than J (true, however, only for positive τ).

Let us now present the first order equation (14) in a time-explicit form. Using Eqs. (17) and (18) we obtain

$$f(\mathbf{v},t+\Delta t)=\frac{1}{\rho}\int_{R^3\times S^2}d\mathbf{w}d\mathbf{n}G\left(\frac{\mathbf{u}\cdot\mathbf{n}}{u},u,\rho\Delta t\right)f(\mathbf{v}',t)f(\mathbf{w}',t), \tag{21}$$

where $F(\mathbf{U},u\mathbf{n})=f(\mathbf{v}',t)f(\mathbf{w}',t)$ is used. The kernel $G(\mu,u,\tau)$ is given by

$$G(\mu,u,\tau)=\sum_{l=0}^{\infty}\frac{2l+1}{4\pi}P_l(\mu)\exp[-\lambda_l(u)\tau], \tag{22}$$

$$\lambda_l(u)=2\pi\int_{-1}^{1}d\mu g(u,\mu)[1-P_l(\mu)]. \tag{23}$$

We note that for a fixed $\rho\Delta t$ the right-hand side of Eq. (21) coincides formally with the gain (positive) term of the collision integral in Eq. (1), having a collisional kernel $G(\mu,u,\rho\Delta t)$. The function $G(\cdot)$ is non-negative; it is the Green function of Eq. (10), and moreover

$$\int_{S^2}d\mathbf{n}G(\boldsymbol{\omega}\cdot\mathbf{n},u,\rho\Delta t)=1. \tag{24}$$

Therefore, the first order equation (21) guarantees positivity of $f(\mathbf{v},t+\Delta t)$ for $f(\mathbf{v},t)\geqslant 0$ and fulfillment of all classical conservation laws. It is now clear that the Nanbu-Babovsky particle method [4] can be used for simulation of Eq. (21) with almost no changes. It is remarkable that Eq. (21) corresponds to the *constant collision frequency*. That is, collisional pairs in numerical realization can be chosen randomly, so that the realization is very simple.

For the sake of generality, we also present the form of Eq. (21) for the case of short-range forces. Since

$$\lim_{l\to\infty}\lambda_l(u)=u\sigma_{\mathrm{tot}}<\infty,$$

Eq. (23) can be transformed into the following form:

$$G(\mu,u,\tau)=\frac{1}{2\pi}\delta(1-\mu)\exp(-u\sigma_{\mathrm{tot}}\tau)+[1-\exp(-u\sigma_{\mathrm{tot}}\tau)]R(\mu,u,\tau),$$

where

$$R(\mu,u,\tau)=\sum_{l=0}^{\infty}\frac{2l+1}{4\pi}P_l(\mu)\frac{\exp[g_l(u)\tau]-1}{\exp[u\sigma_{\mathrm{tot}}\tau]-1}, \tag{25}$$

and

$$g_l(u)=2\pi\int_{-1}^{1}d\mu g(u,\mu)P_l(\mu).$$

The corresponding transformation of Eq. (21) yields

$$f(\mathbf{v},t+\Delta t)=\frac{1}{\rho}\int_{R^3}d\mathbf{w}\left\{f(\mathbf{v},t)f(\mathbf{w},t)\exp(-u\sigma_{\mathrm{tot}}\rho\Delta t)+[1-\exp(-u\sigma_{\mathrm{tot}}\rho\Delta t)]\times\int_{S^2}d\mathbf{n}R\left(\frac{\mathbf{u}\cdot\mathbf{n}}{u},u,\rho\Delta t\right)f(\mathbf{v}'t)f(\mathbf{w}',t)\right\}. \tag{26}$$

It is easy to show that $R(\mu,u,\tau)\geqslant 0$ and

$$2\pi\int_{-1}^{1}d\mu R(\mu,u,\tau)=1. \tag{27}$$

The probabilistic meaning of Eq. (26) is obvious: The collision between particles with velocities $\mathbf{v}$ and $\mathbf{w}$ occurs with a probability of $P_{\mathrm{col}}(\Delta t)=1-\exp(-u\sigma_{\mathrm{tot}}\rho\Delta t)$, and the post-collisional velocities are distributed in accordance with indicatrix $R(\mu,u,\rho\Delta t)$. [Note that $R=(4\pi)^{-1}$ for a hard-sphere molecule.] The simulation method for short-range forces based on Eq. (26) has some advantages compared with the standard scheme [4]; in practical realization of collision simulations, we do not need to introduce an uncertain quantity such as the maximum relative speed. It is also sufficient to decide whether a collision occurs or not by using the probability $P_{\mathrm{col}}(\Delta t)$ for each random collision pair with velocities $(\mathbf{v},\mathbf{w})$. The price we need to pay for this simplification is the calculation of the function $R(\mu,u,\tau)$ for a given intermolecular potential. However, this function has to be calculated only once; moreover, R is unity in the practically most important case of a hard sphere. Our main concern in this paper is the long-range forces, and hence, we now leave the short-range forces.

In the next section we generalize the methodology to the case of mixtures.

IV. EQUATIONS FOR MIXTURES

We consider an n-component mixture of rarefied gases. We denote the distribution function of species α by $f_\alpha(\mathbf{v},t)$. The reduced mass for $\alpha-\beta$ collision is

$$m_{\alpha\beta}=m_\alpha m_\beta/(m_\alpha+m_\beta)\quad(\alpha,\beta=1,2,\ldots,n). \tag{28}$$

Let $\sigma_{\alpha\beta}(u,\theta)$ be the corresponding differential cross section, u standing for relative speed. Then the Boltzmann equations can be written in a form similar to Eqs. (7)–(9):

$$\frac{\partial f_\alpha(\mathbf{v},t)}{\partial t}=\sum_{\beta=1}^{n}\int_{R^3}d\mathbf{w}J_{\alpha\beta}F_{\alpha\beta}(\mathbf{U}_{\alpha\beta},\mathbf{u}), \tag{29}$$

where $\mathbf{u}=\mathbf{v}-\mathbf{w}$, $\mathbf{U}_{\alpha\beta}=(m_\alpha\mathbf{v}+m_\beta\mathbf{w})/(m_\alpha+m_\beta)$, and

$$F_{\alpha\beta}(\mathbf{U}_{\alpha\beta},\mathbf{u})=f_\alpha\left(\mathbf{U}_{\alpha\beta}+\frac{m_{\alpha\beta}}{m_\alpha}\mathbf{u}\right)f_\beta\left(\mathbf{U}_{\alpha\beta}-\frac{m_{\alpha\beta}}{m_\alpha}\mathbf{u}\right)=f_\alpha(\mathbf{v})f_\beta(\mathbf{w}),$$

$$J_{\alpha\beta}F_{\alpha\beta}(\mathbf{U}_{\alpha\beta},\mathbf{u})=\int_{S^2}d\mathbf{n}g_{\alpha\beta}\left(u,\frac{\mathbf{u}\cdot\mathbf{n}}{u}\right)[F_{\alpha\beta}(\mathbf{U}_{\alpha\beta},u\mathbf{n})-F_{\alpha\beta}(\mathbf{U}_{\alpha\beta},\mathbf{u})], \tag{30}$$

with $g_{\alpha\beta}(u,\cos\theta)=u\sigma_{\alpha\beta}(u,\theta)$.

It is obvious that one can easily repeat all steps of Sec. III and obtain an equation similar to Eq. (21). It is, however, convenient to take into account the fact that a typical collision time, $\tau_{\alpha\beta}$, depends strongly on the species of colliding particles. We therefore introduce

$$\overline{g}_{\alpha\beta}=2\pi\int_{-1}^{1}d\mu g_{\alpha\beta}(\langle u_{\alpha\beta}\rangle,\mu)(1-\mu), \tag{31}$$

where $\langle u_{\alpha\beta}\rangle$ is a typical relative speed between particles of species α and β. Now we rewrite Eq. (29) as

$$\frac{\partial f_\alpha}{\partial t}=\sum_{\beta=1}^{n}\overline{g}_{\alpha\beta}\int_{R^3}d\mathbf{w}\hat{J}_{\alpha\beta}F_{\alpha\beta},\quad \hat{J}_{\alpha\beta}=\frac{1}{\overline{g}_{\alpha\beta}}J_{\alpha\beta}.$$

We again use the approximations

$$\frac{\partial f_\alpha}{\partial t}\simeq\frac{f_\alpha(\mathbf{v},t+\Delta t)-f_\alpha(\mathbf{v},t)}{\Delta t},\quad \hat{J}_{\alpha\beta}\simeq\frac{1}{\varepsilon_\alpha}[\exp(\varepsilon_\alpha\hat{J}_{\alpha\beta})-\hat{I}],$$

and put

$$\varepsilon_\alpha=\Delta t\sum_{\gamma=1}^{n}\overline{g}_{\alpha\gamma}\rho_\gamma,\quad \rho_\gamma=\int_{R^3}d\mathbf{v}f_\gamma(\mathbf{v},t)=\text{const}.$$

This yields

$$f_\alpha(\mathbf{v},t+\Delta t)=\sum_{\beta=1}^{n}\pi_{\alpha\beta}\int_{R^3}d\mathbf{w}[\exp(\varepsilon_\alpha\hat{J}_{\alpha\beta})]f_\alpha(\mathbf{v},t)f_\beta(\mathbf{w},t),$$

where

$$\pi_{\alpha\beta}=\overline{g}_{\alpha\beta}\left(\sum_{\gamma=1}^{n}\overline{g}_{\alpha\gamma}\rho_\gamma\right)^{-1},\quad \sum_{\beta=1}^{n}\pi_{\alpha\beta}\rho_\beta=1. \tag{32}$$

Finally, we express the operator exponentials in a time-explicit form analogous to Eq. (21) and obtain

$$f_\alpha(\mathbf{v},t+\Delta t)=\sum_{\beta=1}^{n}\pi_{\alpha\beta}\int_{R^3\times S^2}d\mathbf{w}d\mathbf{n}G_{\alpha\beta}\left(\frac{\mathbf{u}\cdot\mathbf{n}}{u},u,\frac{\Delta t}{\pi_{\alpha\beta}}\right)\times f_\alpha(\mathbf{v}'_{\alpha\beta},t)f_\beta(\mathbf{w}'_{\alpha\beta},t), \tag{33}$$

where $\mathbf{u}=\mathbf{v}-\mathbf{w}$ and

$$\mathbf{v}'_{\alpha\beta}=\frac{m_\alpha\mathbf{v}+m_\beta\mathbf{w}}{m_\alpha+m_\beta}+\frac{m_{\alpha\beta}}{m_\alpha}u\mathbf{n},\quad \mathbf{w}'_{\alpha\beta}=\frac{m_\alpha\mathbf{v}+m_\beta\mathbf{w}}{m_\alpha+m_\beta}-\frac{m_{\alpha\beta}}{m_\beta}u\mathbf{n}, \tag{34}$$

$$G_{\alpha\beta}(\mu,u,\tau)=\sum_{l=0}^{\infty}\frac{2l+1}{4\pi}P_l(\mu)\times\exp\left\{-2\pi\tau\int_{-1}^{1}d\mu g_{\alpha\beta}(u,\mu)\times[1-P_l(\mu)]\right\}. \tag{35}$$

In case of a simple gas, Eq. (33) reduces to Eq. (21). All arguments at the end of Sec. III can be obviously generalized to the case of mixtures. As will be shown later, arbitrariness in the choice of $\langle u_{\alpha\beta}\rangle$ in Eq. (31) plays no essential role because nothing in Eq. (33) depends on $\langle u_{\alpha\beta}\rangle$ (through $\pi_{\alpha\beta}$) for small Δt.

V. SMALL-ANGLE SCATTERING AND COULOMB INTERACTION

We first consider Eq. (21) for a simple gas and assume that the scattering cross section $\sigma(u,\theta)$ is concentrated at small angles near $\theta=0$. This means that the indicatrix $g(u,\mu)$ of Eq. (2) is concentrated near $\mu=1$. We can thus formally approximate the integral in Eq. (23) as

$$\lambda_l(u)\simeq 2\pi\int_{-1}^{1}d\mu g(u,\mu)[1-P_l(1)+(1-\mu)P'_l(1)]=\pi l(l+1)\int_{-1}^{1}d\mu g(u,\mu)(1-\mu), \tag{36}$$

where $P'_l(1)=l(l+1)/2$ is used. This yields the approximate expression of the Green function $G(\mu,u,\tau)$ of Eq. (22):

$$G(\mu,u,\tau)\simeq G^{(L)}(\mu,u,\tau)=\sum_{l=0}^{\infty}\frac{2l+1}{4\pi}P_l(\mu)\exp\left[-\frac{l(l+1)}{2}u\sigma_{\text{tr}}(u)\tau\right], \tag{37}$$

where $\sigma_{\text{tr}}(u)$ is defined by Eq. (3). The superscript in $G^{(L)}(\cdot)$ means that Eq. (21) with the kernel replaced by $G^{(L)}$ approximates the Landau-Fokker-Planck equation [18,19],

$$\frac{\partial f}{\partial t}=\frac{1}{8}\frac{\partial}{\partial v_i}\int_{R^3}d\mathbf{w}u\sigma_{\text{tr}}(u)(u^2\delta_{ij}-u_iu_j)\times\left(\frac{\partial}{\partial v_j}-\frac{\partial}{\partial w_j}\right)f(\mathbf{v})f(\mathbf{w}). \tag{38}$$

For a formal proof of this statement it is enough to note that

$$\exp\left[\frac{\tau}{2}\frac{\partial}{\partial u_i}u\sigma_{\text{tr}}(u)(u^2\delta_{ij}-u_iu_j)\frac{\partial}{\partial u_j}\right]\psi(\mathbf{u})=\int_{S^2}d\mathbf{n}G^{(L)}\left(\frac{\mathbf{u}\cdot\mathbf{n}}{u},u,\tau\right)\psi(u\mathbf{n}), \tag{39}$$

and repeat all steps in Sec. III for Eq. (38). The procedure can be immediately generalized to mixtures: We need only replace $G_{\alpha\beta}$ in Eq. (33) by $G^{(L)}_{\alpha\beta}$, which is given by Eq. (37) after replacing $\sigma_{\text{tr}}(u)$ by

$$\sigma^{\text{tr}}_{\alpha\beta}(u)=2\pi\int_0^\pi d\theta\sigma_{\alpha\beta}(u,\theta)\sin\theta(1-\cos\theta). \tag{40}$$

Let us now consider the most important case of the Coulomb potential,

$$V_{\alpha\beta}(r)=\frac{q_\alpha q_\beta}{4\pi\epsilon_0 r},\quad(\alpha,\beta=1,2,\ldots,n)$$

where r is the distance between two particles with charges q_α and q_β, and ϵ_0 is the permittivity of free space. By the use of the Rutherford formula

$$\sigma_{\alpha\beta}(u,\theta)=\left(\frac{q_\alpha q_\beta}{4\pi\epsilon_0 m_{\alpha\beta}u^2}\right)^2(1-\cos\theta)^{-2},$$

the integral of Eq. (40) with angle cutoff at $\theta=\theta_{\alpha\beta}^{\min}$ results in

$$\sigma_{\alpha\beta}^{\mathrm{tr}}(u)\simeq 4\pi\left(\frac{q_\alpha q_\beta}{4\pi\epsilon_0 m_{\alpha\beta}u^2}\right)^2\ln\Lambda_{\alpha\beta},$$

where the standard approximation

$$\left|\ln\left(\sin\frac{\theta_{\alpha\beta}^{\min}}{2}\right)\right|\simeq\ln\Lambda_{\alpha\beta}=\mathrm{const}$$

is used. The Coulomb logarithm $\ln\Lambda_{\alpha\beta}$ is defined in the usual way. The scattering angle θ is given by $\tan(\theta/2)=|q_\alpha q_\beta|/4\pi\epsilon_0 m_{\alpha\beta}u^2 b$, where b is the impact parameter. Set $\theta=\theta_{\alpha\beta}^{\min}$ at $u^2=\langle u_{\alpha\beta}^2\rangle$ and $b=\lambda_D$, where λ_D is chosen to be the Debye length independent of species and $\langle u_{\alpha\beta}^2\rangle$ is the average of u^2 for $\alpha-\beta$ collisions. Then we have

$$\Lambda_{\alpha\beta}=\frac{4\pi\epsilon_0 m_{\alpha\beta}\langle u_{\alpha\beta}^2\rangle\lambda_D}{|q_\alpha q_\beta|}.$$

We choose $\langle u_{\alpha\beta}^2\rangle$ as

$$\langle u_{\alpha\beta}^2\rangle=\frac{3kT_\alpha}{m_\alpha}+\frac{3kT_\beta}{m_\beta}+(\langle\mathbf{v}_\alpha\rangle-\langle\mathbf{v}_\beta\rangle)^2.$$

This value was evaluated by assuming the Maxwellian distributions for species α and β, where T_α and T_β are the temperatures, and $\langle\mathbf{v}_\alpha\rangle$ and $\langle\mathbf{v}_\beta\rangle$ are the flow velocities. Note that $\Lambda_{\alpha\beta}=\Lambda_{\beta\alpha}$. If $T_\alpha=T_\beta=T$ and $\langle\mathbf{v}_\alpha\rangle=\langle\mathbf{v}_\beta\rangle$, then $\langle u_{\alpha\beta}^2\rangle=3kT/m_{\alpha\beta}$ and hence, $\Lambda_{\alpha\beta}=12\pi\epsilon_0\lambda_D kT/|q_\alpha q_\beta|$. In the case of $|q_\alpha|=|q_\beta|=e$, this $\Lambda_{\alpha\beta}$ is the constant independent of species. For the sake of simplicity, here we set the $\ln\Lambda_{\alpha\beta}$ constant for any α and β and insert $\Lambda_{\alpha\beta}=\Lambda$. However, the extension to the case when $\ln\Lambda$ depends on species is straightforward.

We now formulate the final results for multicomponent plasma. The time evolution of species α is described in the time-explicit form

$$f_\alpha(\mathbf{v},t+\Delta t)=\sum_{\beta=1}^{n}\pi_{\alpha\beta}\int_{R^3\times S^2}d\mathbf{w}d\mathbf{n}D_{\alpha\beta}\times\left(\frac{\mathbf{u}\cdot\mathbf{n}}{u},A_{\alpha\beta}\frac{\Delta t}{u^3}\right)f_\alpha(\mathbf{v}'_{\alpha\beta},t)f_\beta(\mathbf{w}'_{\alpha\beta},t),\tag{41}$$

where $\mathbf{u}=\mathbf{v}-\mathbf{w}$, $\mathbf{v}'_{\alpha\beta}$ and $\mathbf{w}'_{\alpha\beta}$ are defined by Eq. (34), and

$$\pi_{\alpha\beta}=\left[\sum_{\gamma=1}^{n}\rho_\gamma\frac{\langle u_{\alpha\beta}\rangle^3 m_{\alpha\beta}^2 q_\gamma^2}{\langle u_{\alpha\gamma}\rangle^3 m_{\alpha\gamma}^2 q_\beta^2}\right]^{-1},$$

$$A_{\alpha\beta}=\frac{2\pi}{\pi_{\alpha\beta}}\left(\frac{q_\alpha q_\beta}{4\pi\epsilon_0 m_{\alpha\beta}}\right)^2\ln\Lambda,\tag{42}$$

$$D_{\alpha\beta}(\mu,\tau)=\sum_{l=0}^{\infty}\frac{2l+1}{4\pi}P_l(\mu)\exp[-l(l+1)\tau].\tag{43}$$

The simplest estimate of $\langle u_{\alpha\beta}\rangle$ can be obtained by assuming an equilibrium plasma with temperature T:

$$\langle u_{\alpha\beta}\rangle=(8kT/\pi m_{\alpha\beta})^{1/2},\tag{44}$$

k being the Boltzmann constant. By use of Eq. (44), the final form of $\pi_{\alpha\beta}$ reads as

$$\pi_{\alpha\beta}=\left[\sum_{\gamma=1}^{n}\rho_\gamma\frac{q_\gamma^2}{q_\beta^2}\sqrt{\frac{m_{\alpha\beta}}{m_{\alpha\gamma}}}\right]^{-1}.\tag{45}$$

In the simplest case of charge-neutral hydrogen plasma consisting of electrons ($\alpha=e$) and protons ($\alpha=i$), we obtain

$$\rho_e=\rho_i(=\rho),\quad m_{ii}=\frac{m_i}{2},\quad m_{ee}=\frac{m_e}{2},\quad m_{ie}=m_{ei}\simeq m_e,$$

$$q_i^2=q_e^2(=e^2),\quad \pi_{ii}^{-1}=\rho\left(1+\frac{1}{\gamma}\right),\quad \pi_{ie}^{-1}=\rho(1+\gamma),$$

$$\pi_{ee}^{-1}=\rho\left(1+\frac{1}{\sqrt{2}}\right),\quad \pi_{ei}^{-1}=\rho(1+\sqrt{2}),\quad \gamma^2=\frac{2m_e}{m_i},$$

$$A_{ii}=8\pi\rho\left(1+\frac{1}{\gamma}\right)\frac{e^4}{m_i^2}\ln\Lambda,\quad A_{ie}=2\pi\rho(1+\gamma)\frac{e^4}{m_e^2}\ln\Lambda,$$

$$A_{ee}=8\pi\rho\left(1+\frac{1}{\sqrt{2}}\right)\frac{e^4}{m_i^2}\ln\Lambda,\quad A_{ei}=2\pi\rho(1+\sqrt{2})\frac{e^4}{m_e^2}\ln\Lambda.\tag{46}$$

These equations give all coefficients in Eq. (41) for $\alpha=i$ or e. It should be noted, however, that any other reasonable choice of $\pi_{\alpha\beta}$ satisfying the conditions

$$\sum_{\beta=1}^{n}\pi_{\alpha\beta}\rho_\beta=1,\quad(\alpha=1,2,\ldots,n),\tag{47}$$

is also allowable.

VI. SIMPLIFIED SCHEMES AND COMPARISON WITH THE PREVIOUS APPROACH

In this section, we discuss a possible way of simplifying Eq. (43). A disadvantage of the numerical scheme based on Eqs. (41)–(43) is that the probability density function $D(\mu,\tau)$ is rather complicated (suffix $\alpha\beta$ is omitted). At each time step one needs to obtain a random sample of the quantity $\mu(\tau)$ distributed in $[-1,1]$. It is therefore desirable to deal with a simpler function $D_*(\mu,\tau)$ approximating Eq. (43). For this purpose, we first note that Eq. (41) is correct only with an accuracy of $O(\Delta t)$, as is clear from its derivation. Hence, the function (43) can be replaced by any other function $D_*(\mu,\tau)$ satisfying the following conditions:

$$\text{(a)}\quad D_*(\mu,\tau)\geqslant 0,\quad 2\pi\int_{-1}^{1} d\mu D_*(\mu,\tau)=1, \tag{48a}$$

$$\text{(b)}\quad \lim_{\tau\to 0} D_*(\mu,\tau)=\frac{1}{2\pi}\,\delta(1-\mu), \tag{48b}$$

$$\text{(c)}\quad \lim_{\tau\to 0}\frac{2\pi}{\tau}\int_{-1}^{1} d\mu[D_*(\mu,\tau)-D(\mu,\tau)]P_l(\mu)=0. \tag{48c}$$

Equation (48c) must hold for all $l=1,2,\ldots$. We begin with two remarks.

Remark 1. Replacing the kernel by its first order approximation is allowable not only in Eq. (41) for plasmas but also in Eq. (33) for general long-range forces, provided that conditions (48a)–(48c) are satisfied by replacing $D(\mu,\tau)$ by $G_{\alpha\beta}(\mu,u,\tau)$ and $D_*(\mu,\tau)$ by $G^*_{\alpha\beta}(\mu,u,\tau)$, which is an approximation of $G_{\alpha\beta}(\mu,u,\tau)$. As we stressed in the Introduction, the starting point for the present paper is the method proposed in Ref. [16] on the basis of intuitive physical considerations. We are now able to show that the approach of Ref. [16] is really the solution method of the Landau-Fokker-Planck equation in the limit of $\Delta t\to 0$. Roughly speaking, the previous method [16] is equivalent to a numerical realization of the Markov process of Eq. (41) (we ignore an irrelevant choice of $\pi_{\alpha\beta}$ and some other details), where $D(\mu,\tau)$ is approximated by the function

$$D_*(\mu,\tau)=\frac{A}{4\pi\sinh A}\exp(\mu A), \tag{49}$$

with $A=A(\tau)$ satisfying the equation

$$\coth A-\frac{1}{A}=e^{2\tau}. \tag{50}$$

Remark 2. To completely clarify the comparison with Ref. [16], it should be noted that the function $D_*(\cos\chi_N,s/2)$ corresponds to $f(\chi_N)$ for fixed parameter s in the notations of Ref. [16]. It is sufficient for our purpose to show that function (49) does satisfy conditions (48a)–(48c). The limit $\tau\to 0$ corresponds to the limit $A\to\infty$; moreover, $A(\tau)\simeq(2\tau)^{-1}$ as $\tau\to 0$ in accordance with Eq. (50). Therefore, conditions (48a) and (48b) are obviously fulfilled. Condition (48c) can be written in the following equivalent form:

$$\lim_{\tau\to 0}\frac{2\pi}{\tau}\int_{-1}^{1} d\mu D_*(\mu,\tau)[1-P_l(\mu)] = l(l+1),\quad (l=1,2,\ldots). \tag{51}$$

We substitute Eq. (49) into the left-hand side of Eq. (51) and consider the limit $\tau\to 0$ (note that $2A\tau\to 1$ as $\tau\to 0$). This yields

$$\begin{aligned}\frac{1}{2\tau^2}\int_{-1}^{1} d\mu[1-P_l(\mu)]\exp\left(-\frac{1-\mu}{2\tau}\right) &= \frac{1}{\tau}\int_0^{1/\tau} dx e^{-x}[1-P_l(1-2x\tau)]\\ &\simeq \lim_{\tau\to 0} 2P_l'(1)\int_0^{1/\tau} dx x e^{-x}\\ &= 2P_l'(1)=l(l+1).\end{aligned}$$

Hence, all conditions (48a)–(48c) are fulfilled. Therefore, the scheme presented in Ref. [16] approximates the Landau-Fokker-Planck equation. Let us further develop our idea. To approximate $D(\mu,\tau)$ we need not always solve Eq. (50) for $A(\tau)$; it is enough if only condition (48c) is satisfied. To do this one can use the following simple lemma.

Lemma. Conditions (48a)–(48c) are fulfilled for any function

$$D_*(\mu,\tau)=\psi\left(\frac{1-\mu}{2\tau}\right)\left[4\pi\tau\int_0^{1/\tau} dx\,\psi(x)\right]^{-1},$$

where $\psi(x)$ satisfies $\psi(x)\geqslant 0$ for $x>0$ and

(i) $\int_0^\infty dx\,\psi(x)=\int_0^\infty dx\,x\,\psi(x)<\infty$,

(ii) $\lim_{\tau\to 0}\tau\int_{1/\tau}^\infty dx x^n\psi(x)=0$, $(n=2,3,\ldots)$.

Proof. It is sufficient to prove Eq. (48c). Let us write the left-hand side of Eq. (51) as $\lim_{\tau\to 0} Z_l(\tau)$, where

$$Z_l(\tau)=\frac{2\pi}{\tau}\int_{-1}^{1} d\mu D_*(\mu,\tau)[1-P_l(\mu)],$$

and note that

$$\int_{-1}^{1} d\mu\,\psi\left(\frac{1-\mu}{2\tau}\right)P_l(\mu)=2\tau\int_0^{1/\tau} dx\,\psi(x)P_l(1-2x\tau).$$

Hence, as $\tau\to 0$, we have

$$Z_l(\tau)=\frac{\int_0^{1/\tau} dx\,\psi(x)[1-P_l(1-2x\tau)]}{\tau\int_0^{1/\tau} dx\,\psi(x)}\to 2P_l'(1)=l(l+1),$$

as a consequence of conditions (i) and (ii). The lemma has been proven.

The simplest function $\psi(x)$ satisfying conditions (i) and (ii) is e^{-x} or $\delta(1-x)$. The corresponding kernels are

$$D_*^{(1)}(\mu,\tau)=[4\pi\tau(1-e^{-1/\tau})]^{-1}\exp\left(-\frac{1-\mu}{2\tau}\right),$$

$$D_*^{(2)}(\mu,\tau)=\frac{1}{2\pi}\,\delta[\mu-\nu(\tau)],$$

where $\nu(\tau)=1-2\tau$ for $0\leqslant\tau\leqslant 1$ and $\nu(\tau)=-1$ for $\tau>1$. These kernels can be used in Eq. (41) to approximate the Landau-Fokker-Planck equation with an accuracy of $O(\Delta t)$. Thus, there is no need to use the complicated exact kernel of Eq. (43), or even to use the simplified kernel of Eq. (49) given in Ref. [16]. The simplest choice is, from a practical point of view, the kernel $D_*^{(2)}(\mu,\tau)$. For this kernel, a ran-

dom sample of the direction $\mathbf{n}$ of the postcollisional relative velocity $\mathbf{u}'(=u\mathbf{n}=\mathbf{v}'-\mathbf{w}')$ in Eq. (41) has the following value in the spherical coordinates system (θ,φ) with the polar axis directed to the precollisional relative velocity $\mathbf{u}$: $\theta=\arccos\nu(\tau)$ and $\varphi=2\pi r$, where r is a random number uniformly distributed in (0,1). We therefore need only one random number to simulate the collision.

As already mentioned in *Remark 1*, a similar simplification can be introduced in the scheme for the Boltzmann equation for general long-range forces. This task is, however, less trivial and we do not discuss it in the present paper.

VII. ALGORITHM OF PARTICLE COLLISIONS

We can derive the collision algorithm from Eq. (41). In the Monte Carlo simulation a set of random samples $\{\mathbf{v}_{\alpha1},\mathbf{v}_{\alpha2},\ldots\}$ is employed in place of the velocity distribution function $f_\alpha(\mathbf{v},t)$. The relation between $f_\alpha(\mathbf{v},t)$ and the set is in Ref. [2]

$$f_\alpha(\mathbf{v},t)=\frac{\rho_\alpha}{N_\alpha}\sum_{i=1}^{N_\alpha}\delta(\mathbf{v}-\mathbf{v}_{\alpha i}), \tag{52}$$

where N_α is the number of samples and $\mathbf{v}_{\alpha i}$ is called the velocity of particle αi at time t. Similarly, for species β we write

$$f_\beta(\mathbf{w},t)=\frac{\rho_\beta}{N_\beta}\sum_{j=1}^{N_\beta}\delta(\mathbf{w}-\mathbf{v}_{\beta j}). \tag{53}$$

Substitution of Eqs. (52) and (53) into Eq. (41) yields

$$\frac{1}{\rho_\alpha}f_\alpha(\mathbf{v},t+\Delta t)=\frac{1}{N_\alpha}\sum_{i=1}^{N_\alpha}Q_{\alpha i}(\mathbf{v}), \tag{54}$$

where

$$Q_{\alpha i}(\mathbf{v})=\sum_{\beta=1}^{n}\pi_{\alpha\beta}\rho_\beta\left(\frac{1}{N_\beta}\sum_{j=1}^{N_\beta}Q_{\alpha i,\beta j}(\mathbf{v})\right), \tag{55}$$

$$\begin{aligned}Q_{\alpha i,\beta j}(\mathbf{v})&=\int_{R^3\times S^2}d\mathbf{w}d\mathbf{n}D_{\alpha\beta}\left(\frac{\mathbf{u}\cdot\mathbf{n}}{u},A_{\alpha\beta}\frac{\Delta t}{u^3}\right)\\&\quad\times\delta(\mathbf{v}'_{\alpha\beta}-\mathbf{v}_{\alpha i})\,\delta(\mathbf{w}'_{\alpha\beta}-\mathbf{v}_{\beta j}).\end{aligned} \tag{56}$$

The function $Q_{\alpha i}(\mathbf{v})$ in Eq. (54) can be interpreted as the probability density function of particle αi at time $t+\Delta t$.

Let us rearrange Eq. (56). Using

$$Q_{\alpha i,\beta j}(\mathbf{v}_1)=\int_{R^3}d\mathbf{v}\,\delta(\mathbf{v}-\mathbf{v}_1)Q_{\alpha i,\beta j}(\mathbf{v}),$$

we have

$$\begin{aligned}Q_{\alpha i,\beta j}(\mathbf{v}_1)&=\int_{R^3\times R^3\times S^2}d\mathbf{v}d\mathbf{w}d\mathbf{n}D_{\alpha\beta}\left(\frac{\mathbf{u}\cdot\mathbf{n}}{u},A_{\alpha\beta}\frac{\Delta t}{u^3}\right)\\&\quad\times\delta(\mathbf{v}'_{\alpha\beta}-\mathbf{v}_{\alpha i})\,\delta(\mathbf{w}'_{\alpha\beta}-\mathbf{v}_{\beta j})\,\delta(\mathbf{v}-\mathbf{v}_1),\\&=\int_{R^3\times R^3\times S^2}d\mathbf{v}d\mathbf{w}d\mathbf{n}D_{\alpha\beta}\left(\frac{\mathbf{u}\cdot\mathbf{n}}{u},A_{\alpha\beta}\frac{\Delta t}{u^3}\right)\delta(\mathbf{v}-\mathbf{v}_{\alpha i})\\&\quad\times\delta(\mathbf{w}-\mathbf{v}_{\beta j})\,\delta(\mathbf{v}'_{\alpha\beta}-\mathbf{v}_1),\\&=\int_{S^2}d\mathbf{n}D_{\alpha\beta}\left(\frac{\mathbf{u}_{ij}\cdot\mathbf{n}}{u_{ij}},A_{\alpha\beta}\frac{\Delta t}{u_{ij}^3}\right)\delta(\mathbf{v}_1-\mathbf{v}'_{ij}),\end{aligned} \tag{57}$$

where $\mathbf{u}_{ij}=\mathbf{v}_{\alpha i}-\mathbf{v}_{\beta j}$,

$$\mathbf{v}'_{ij}=\mathbf{W}_{ij}+M_\beta u_{ij}\mathbf{n}, \tag{58}$$

$\mathbf{W}_{ij}=(m_\alpha\mathbf{v}_{\alpha i}+m_\beta\mathbf{v}_{\beta j})/(m_\alpha+m_\beta)$, and $M_\beta=m_\beta/(m_\alpha+m_\beta)$. The second equation of Eq. (57) can be obtained using the standard transformation of exchanging precollisional velocities for postcollisional ones. Now we set $\mathbf{v}_1=\mathbf{v}$ in Eq. (57) and evaluate the integral:

$$\begin{aligned}Q_{\alpha i,\beta j}(\mathbf{v})&=2\int_{R^3}d\mathbf{k}\delta(k^2-1)D_{\alpha\beta}\left(\frac{\mathbf{u}_{ij}\cdot\mathbf{k}}{u_{ij}},A_{\alpha\beta}\frac{\Delta t}{u_{ij}^3}\right)\\&\quad\times\delta(\mathbf{v}-\mathbf{W}_{ij}-M_\beta u_{ij}\mathbf{k}),\\&=D_{\alpha\beta}\left(\frac{\mathbf{u}_{ij}\cdot\mathbf{u}'}{u_{ij}^2},A_{\alpha\beta}\frac{\Delta t}{u_{ij}^3}\right)M_\beta^{-3}u_{ij}^{-2}\delta(u'-u_{ij}),\end{aligned} \tag{59}$$

where $\mathbf{u}'=(\mathbf{v}-\mathbf{W}_{ij})/M_\beta$. If we write $\mathbf{n}'=\mathbf{u}'/u'$, we have $d\mathbf{v}=M_\beta^3u'^2du'd\mathbf{n}'$, $d\mathbf{n}'$ being an element of the solid angle. From Eq. (59), we then have

$$Q_{\alpha i,\beta j}(\mathbf{v})d\mathbf{v}=D_{\alpha\beta}\left(\frac{\mathbf{u}_{ij}\cdot\mathbf{n}'}{u_{ij}},A_{\alpha\beta}\frac{\Delta t}{u_{ij}^3}\right)\delta(u'-u_{ij})du'd\mathbf{n}'. \tag{60}$$

Integration of $Q_{\alpha i,\beta j}(\mathbf{v})$ over the whole $\mathbf{v}$ yields unity; $Q_{\alpha i,\beta j}(\mathbf{v})$ is the probability density function.

How to determine the velocity of particle αi at $t+\Delta t$ is now clear from Eqs. (55) and (60). First of all, note that the probability density $Q_{\alpha i}(\mathbf{v})$ of particle αi does not take the form for short-range forces such as [2]

$$[1-P_{\mathrm{col}}(\Delta t)]\delta(\mathbf{v}-\mathbf{v}_{\alpha i})+P_{\mathrm{col}}(\Delta t)Q_{\alpha i}(\mathbf{v}),$$

where $P_{\mathrm{col}}(\Delta t)$ is the collision probability of particle αi in time Δt. The first term represents no collision. Lack of the first term means that in Coulomb collisions, $P_{\mathrm{col}}(\Delta t)$ is unity however small Δt is; every particle collides in Δt. Second, note that Eq. (55) satisfies

$$\int_{R^3}Q_{\alpha i}(\mathbf{v})d\mathbf{v}=\sum_{\beta=1}^{n}\pi_{\alpha\beta}\rho_\beta=1.$$

This means that the collision partner of particle αi is a particle of species β with a probability of $\pi_{\alpha\beta}\rho_\beta$. Let β be a species sampled from the distribution of $\pi_{\alpha\beta}\rho_\beta$. Third, note then that

$$\frac{1}{N_\beta}\int_{R^2}Q_{\alpha i,\beta j}(\mathbf{v})d\mathbf{v}=\frac{1}{N_\beta}. \tag{61}$$

Equation (55) shows that the value of Eq. (61) represents the probability that under the condition that particle αi collides with some particle in species β, the collision partner is the specific particle βj. Since Eq. (61) is independent of j, all particles $\beta 1$, $\beta 2, \ldots$ are equally probable as the partner of particle αi; we have only to randomly sample a partner from N_β particles. Let βj be the partner, whose velocity is $\mathbf{v}_{\beta j}$ at time t. Lastly, the integrand of Eq. (61), which is given in Eq. (60), gives the probability that the velocity of particle αi at $t+\Delta t$ is included in volume $d\mathbf{v}$ centered at $\mathbf{v}$. The velocity of particle αi is given by

$$\mathbf{v}_{\alpha i}(t+\Delta t)=\mathbf{W}_{ij}+M_\beta u'\mathbf{n}',$$

where $\mathbf{W}_{ij}=[m_\alpha \mathbf{v}_{\alpha i}(t)+m_\beta \mathbf{v}_{\beta j}(t)]/(m_\alpha+m_\beta)$, $u'=|\mathbf{v}_{\alpha i}(t)-\mathbf{v}_{\beta j}(t)|$, and the direction $\mathbf{n}'$ of $\mathbf{u}'$ is to be sampled from the probability density $D_{\alpha\beta}$ in Eq. (60), where $u_{ij}=|\mathbf{v}_{\alpha i}(t)-\mathbf{v}_{\beta j}(t)|$.

We have described a method to determine the velocity of one particle αi at $t+\Delta t$. In the particle simulation of plasmas, the velocities of all particles $\{\alpha 1,\alpha 2,\ldots,\alpha N_\alpha\}$, $\{\beta 1,\beta 2,\ldots,\beta N_\beta\}$, ... should be calculated simultaneously at each time step. For the sake of simplicity, let us consider the plasma consisting of species α and β. We have to calculate all $\alpha-\alpha$, $\beta-\beta$, and $\alpha-\beta$ collisions in time Δt. Such a case can be treated by modifying the collision algorithm for one particle. Of course, the simplest method to determine the particle velocities at $t+\Delta t$ is to use the one particle algorithm for any particle. Using Eq. (41), one can, in fact, verify that the resulting momentum and energy of the particle system consisting of all species are conserved when one particle algorithm is used. Since the numbers of simulated particles, N_α and N_β, are finite, however, the momentum and energy show statistical fluctuations around the expectations. To avoid such fluctuations, it is necessary to consider pairwise collisions and to satisfy the conservation laws in each collision. This is done as follows. Note, however, that the strategy of pairwise collisions is based on a physical idea rather than on the kinetic equation. Let us count the average numbers of $\alpha-\alpha$, $\beta-\beta$, and $\alpha-\beta$ collisions in time Δt. First, note that for a binary mixture, Eq. (32) gives

$$N_\alpha \pi_{\alpha\alpha}\rho_\alpha+N_\alpha \pi_{\alpha\beta}\rho_\beta=N_\alpha, \tag{62a}$$

$$N_\beta \pi_{\beta\alpha}\rho_\alpha+N_\beta \pi_{\beta\beta}\rho_\beta=N_\beta. \tag{62b}$$

Equation (62a) means that N_α particles of species α are divided into two groups: $N_\alpha \pi_{\alpha\alpha}\rho_\alpha$ particles collide with particles α and $N_\alpha \pi_{\alpha\beta}\rho_\beta$ particles collide with particles β. Similarly, $N_\beta \pi_{\beta\alpha}\rho_\alpha$ in Eq. (62b) is the number of particles β which collide with particles α. Introduction of the concept of pairwise collisions requires that the number of $\alpha-\beta$ collisions is unique, i.e.,

$$N_\alpha \pi_{\alpha\beta}\rho_\beta=N_\beta \pi_{\beta\alpha}\rho_\alpha. \tag{63}$$

The number densities are expressed as $\rho_\alpha=CN_\alpha/V_c$ and $\rho_\beta=CN_\beta/V_c$, where V_c is the cell volume and C is the weight (one simulated particle represents C real particles). Substitution of ρ_α and ρ_β into Eq. (63) yields $\pi_{\alpha\beta}=\pi_{\beta\alpha}$. This is a strong condition for the choice of $\pi_{\alpha\beta}$. In fact, $\pi_{\alpha\beta}$ defined by Eq. (32) does not satisfy $\pi_{\alpha\beta}=\pi_{\beta\alpha}$. The case of $\pi_{\alpha\beta}\neq\pi_{\beta\alpha}$ is treated in Sec. VIII.

There is one more reason for the necessity of symmetrical $\pi_{\alpha\beta}$. For a pairwise collision of particles αi and βj, the postcollisional velocities are given by

$$\mathbf{v}_{\alpha i}(t+\Delta t)=\mathbf{W}_{ij}+M_\beta u_{ij}\mathbf{n}', \tag{64a}$$

$$\mathbf{v}_{\beta j}(t+\Delta t)=\mathbf{W}_{ij}-M_\alpha u_{ij}\mathbf{n}'. \tag{64b}$$

Of course, the same vector $\mathbf{n}'$ must be used in both Eqs. (64a) and (64b). The probability density function of $\mathbf{n}'$ in Eq. (64a) is $D_{\alpha\beta}$ in Eq. (60). However, the probability density function of $\mathbf{n}'$ in Eq. (64b) is

$$D_{\beta\alpha}\left(\frac{\mathbf{u}_{ij}\cdot\mathbf{n}'}{u_{ij}},A_{\beta\alpha}\frac{\Delta t}{u_{ij}^3}\right).$$

The two probability densities should coincide for a given Δt because $\mathbf{n}'$ in Eqs. (64a) and (64b) is identical. The condition $D_{\alpha\beta}=D_{\beta\alpha}$ requires $A_{\alpha\beta}=A_{\beta\alpha}$ and hence, $\pi_{\alpha\beta}=\pi_{\beta\alpha}$ results from Eq. (42). The simplest form of $\pi_{\alpha\beta}$ that satisfies $\pi_{\alpha\beta}=\pi_{\beta\alpha}$ and Eq. (47) is

$$\pi_{\alpha\beta}=\left(\sum_{\gamma=1}^{n}\rho_\gamma\right)^{-1}=\text{const} \tag{65}$$

If we replace $\pi_{\alpha\beta}$ in Eq. (42) by the constant of Eq. (65), all equations hold as they stand. Let us use Eq. (65) in the following pairwise collision algorithm. Set $\pi_{\alpha\beta}=\rho^{-1}$.

(i) Find randomly $N_{\alpha\beta}(\equiv N_\alpha\rho_\beta/\rho)$ particles from species α and the same number of particles from species β without replacement. Calculate $\alpha-\beta$ collisions of $N_{\alpha\beta}$ pairs. The postcollisional velocities $\mathbf{v}_{\alpha i}(t+\Delta t)$ and $\mathbf{v}_{\beta j}(t+\Delta t)$ are given by Eqs. (64a) and (64b).

(ii) Choose $N_{\alpha\alpha}[=(N_\alpha-N_{\alpha\beta})/2]$ pairs randomly without replacement from the particles α unused in step (i). Calculate $\alpha-\alpha$ collisions of these pairs.

(iii) Choose $N_{\beta\beta}[=(N_\beta-N_{\alpha\beta})/2]$ pairs randomly without replacement from the particles β unused in step (i). Calculate $\beta-\beta$ collisions of these pairs.

The collisions are calculated in the order of $\alpha-\beta$, $\alpha-\alpha$, and $\beta-\beta$. The order is arbitrary because every particle collides only once in Δt. In practical simulations, the Cartesian components of postcollisional velocities are necessary. They can be found in Ref. [22].

VIII. WEIGHT ALGORITHM

The choice of Eq. (45) is quite natural from the physical point of view, although $\pi_{\alpha\beta}\neq\pi_{\beta\alpha}$. Hence, it is significant to give the pairwise collision algorithm for $\pi_{\alpha\beta}\neq\pi_{\beta\alpha}$. Also, the argument concerning this algorithm makes it possible to treat the case when the weight of a simulated particle depends on the species. In multicharged plasmas, electron density is several times larger than ion density; if we use a larger weight for electrons, we can make the number of simulated electrons nearly equal to the number of simulated ions, thus reducing the computation time.

First, we consider the case of equal weights, $C_\alpha=C_\beta=C$. Since $\pi_{\alpha\beta}\neq\pi_{\beta\alpha}$ is assumed, Eq. (63) does not hold for

$\alpha \neq \beta$. We consider the case of $\pi_{\alpha\beta} > \pi_{\beta\alpha}$ without loss of generality. Let us write

$$N'_\alpha = N_\alpha \pi_{\alpha\beta} \rho_\beta, \quad N'_\beta = N_\beta \pi_{\beta\alpha} \rho_\alpha. \tag{66}$$

Clearly, N'_α is larger than N'_β for $\pi_{\alpha\beta} > \pi_{\beta\alpha}$. Let us modify step (i) in the algorithm of Sec. VII as follows. To facilitate understanding, we consider the case of $N'_\alpha = 7$ and $N'_\beta = 3$. First note that

$$D_{\alpha\beta}\left(\frac{\mathbf{u}_{ij}\cdot\mathbf{n}'}{u_{ij}}, A_{\alpha\beta}\frac{\Delta t}{u_{ij}^3}\right) = D_{\beta\alpha}\left(\frac{\mathbf{u}_{ij}\cdot\mathbf{n}'}{u_{ij}}, A_{\beta\alpha}\frac{\Delta t'}{u_{ij}^3}\right) \tag{67}$$

for $\Delta t' = (A_{\alpha\beta}/A_{\beta\alpha})\Delta t = (\pi_{\beta\alpha}/\pi_{\alpha\beta})\Delta t$. This means that if $\mathbf{n}'$ in Eqs. (64a) and (64b) is sampled from the probability density function $D_{\alpha\beta}$, the time increment Δt in Eq. (64b) must be replaced by $\Delta t'$. A similar notion was used in Ref. [23]. We now consider $7(=N'_\alpha)$ collisions between particles α and β. However, we have only $3(=N'_\beta)$ particles of species β. Let $(\alpha 1, \alpha 2, \ldots, \alpha 7)$ and $(\beta 1, \beta 2, \beta 3)$ be sets of randomly sampled particles, respectively. Noting that $7 = 3 + 3 + 1$, we first calculate $(\alpha 1, \beta 1)$, $(\alpha 2, \beta 2)$, and $(\alpha 3, \beta 3)$ collisions, next $(\alpha 4, \beta 1')$, $(\alpha 5, \beta 2')$, and $(\alpha 6, \beta 3')$ collisions, and lastly a $(\alpha 7, \beta 1'')$ collision, where a single prime means the second collision and double primes the third collision. Of course, the precollisional velocity of $\beta 1'$ is the postcollisional velocity of $\beta 1$, and the precollisional velocity of $\beta 1''$ is the postcollisional velocity of $\beta 1'$. The mean time increment of particles α is trivial, i.e., $N'_\alpha \Delta t / N'_\alpha = \Delta t$. Since the total number of collisions is N'_α, the mean time increment of N'_β particles is $N'_\alpha \Delta t' / N'_\beta = N'_\alpha (\pi_{\beta\alpha}/\pi_{\alpha\beta}) \Delta t / N'_\beta = \Delta t$. Thus, we see that the collision algorithm described results in the same time increment for species α and β.

The treatment of $\alpha - \alpha$ and $\beta - \beta$ collisions is the same as steps (ii) and (iii) in Sec. VII. Some remarks are necessary for the case when $N_{\alpha\alpha}(=N_\alpha - N'_\alpha)$ or $N_{\beta\beta}(=N_\beta - N'_\beta)$ is an odd number. As an example, we consider the case of $N_{\alpha\alpha} = 5$ with $N_\alpha = 12$ and $N'_\alpha = 7$. Let $(\alpha 1, \alpha 2, \ldots, \alpha 12)$ be a random array of particles α, where $(\alpha 8, \alpha 9, \alpha 10, \alpha 11, \alpha 12)$ are unused particles in the $\alpha - \beta$ collision calculation. We calculate three collisions of pairs $(\alpha 8, \alpha 9)$, $(\alpha 10, \alpha 11)$, $(\alpha 12, \alpha 8')$ using the function $D_{\alpha\alpha}$, where $\alpha 8'$ denotes the second collision of particle $\alpha 8$. The mean time increment of particles α is $2\Delta \times t 3/5$, i.e., $2\Delta t[(N_{\alpha\alpha}+1)/2]/N_{\alpha\alpha} = [(N_{\alpha\alpha}+1)/N_{\alpha\alpha}]\Delta t$. This is larger than Δt because of the second collision of particle $\alpha 8$. The physical time of the whole particle system should be advanced by a given time step Δt_p. Clearly, this is satisfied if we set $\Delta t = [N_{\alpha\alpha}/(N_{\alpha\alpha}+1)]\Delta t_p$ in the function $D_{\alpha\alpha}$ for odd $N_{\alpha\alpha}$. For even $N_{\alpha\alpha}$, no such a correction is needed, i.e., $\Delta t = \Delta t_p$.

Next let us consider the case of different weights, $C_\alpha \neq C_\beta$. A collision of simulated particles α and β represents collisions of C_α real particles α with C_β real particles. Let us consider the case of $C_\alpha = 5$ and $C_\beta = 3$; only three pairwise collisions can be realized. This can be described through probability theory: Simulated particle α undergoes a collision with probability $C_\beta/\max(C_\alpha, C_\beta)[=3/5]$ and simulated particle β does so with probability $C_\alpha/\max(C_\alpha, C_\beta)[=1]$. We now calculate mean time increments. Equations (66) take the form

$$N'_\alpha = N_\alpha N_\beta \frac{\pi_{\alpha\beta} C_\beta}{V_c}, \quad N'_\beta = N_\alpha N_\beta \frac{\pi_{\beta\alpha} C_\alpha}{V_c}. \tag{68}$$

Let us consider the case of $N'_\alpha > N'_\beta$. As in the case of $C_\alpha = C_\beta$, we consider N'_α pairwise collisions between particles α and β; some particles β collide twice or more because $N'_\alpha > N'_\beta$. We use $D_{\alpha\beta}$ in Eq. (67) to make a random sample of $\mathbf{n}'$. Then the mean time increment of real particles α is

$$\Delta t \frac{C_\alpha C_\beta}{\max(C_\alpha, C_\beta)} N'_\alpha \frac{1}{N'_\alpha C_\alpha} = \frac{C_\beta}{\max(C_\alpha, C_\beta)} \Delta t, \tag{69a}$$

where $C_\alpha C_\beta / \max(C_\alpha, C_\beta)$ is the number of real particles α that have collided in one $\alpha - \beta$ collision of simulated particles. Similarly, the mean time increment of real particles β is

$$\Delta t' \frac{C_\beta C_\alpha}{\max(C_\alpha, C_\beta)} N'_\alpha \frac{1}{N'_\beta C_\beta} = \frac{C_\beta}{\max(C_\alpha, C_\beta)} \Delta t, \tag{69b}$$

where $\Delta t' = (\pi_{\beta\alpha}/\pi_{\alpha\beta})\Delta t$ and Eq. (68) were employed. We see that the collision algorithm results in the same time increment for two species. As before, we have only to choose Δt in the function $D_{\alpha\beta}$ of Eq. (67) as

$$\Delta t = \frac{\max(C_\alpha, C_\beta)}{C_\beta} \Delta t_p.$$

Then the physical time of the system is advanced by a given value Δt_p after all $\alpha - \beta$ collision calculations.

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