Non-Boltzmann classical correction to the velocity auto-correlation function for isotropic scattering in two dimensions

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The classical correction to the velocity autocorrelation function of noninteracting particles due to memory effects, which are beyond the Boltzmann equation, is calculated both analytically and numerically for the case of isotropic scattering in two dimensions.

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I. INTRODUCTION

Some forty years ago a number of pioneering theoretical works appeared,[1–7] which were devoted to the calculation of the memory-effect (non-Markovian) corrections to the kinetic coefficients and to the velocity autocorrelation function, through which they can be expressed. It was shown that such quantities as the diffusion coefficient, the electrical conductivity, viscosity, etc., cannot be expanded in powers of density, as was assumed previously. Later, it was also demonstrated that the velocity autocorrelation function (which we abbreviate below as "correlation function") does not decay exponentially at large times, as the Boltzmann equation predicts, but rather contains a slow power-law tail.[8–10]

These important deviations from the conventional picture based on the Boltzmann equation are due to memory effects neglected in the Boltzmann approach. For the case of noninteracting particles performing diffusion in a static random potential field these effects are due to returns of the particle to previously visited regions. In the two-dimensional case it was shown by Ernst and Wejland[9] that, because of returns, for times t much greater than the mean free flight time τ, the correlation function has a negative tail decaying as $1/t^2$. Bruin[10] has performed numerical calculations for scattering by hard disks, which showed that this asymptotic behavior for $t \gg \tau$ may appear only at very long times, it is not reached even at $t \simeq 10\tau$.

Returns after a single collision [see Fig. 1(a)] are important at $t \lesssim \tau$. For $t \ll \tau$ they give a contribution to the probability of return increasing as $1/t$. This, in turn, leads to a nonanalytical in the small parameter $d/l = Nd^2$ correction to the diffusion coefficient on the order of $(d/l)\ln(l/d)$, where d is the effective scattering diameter, $l = (Nd)^{-1}$ is the mean free path, and N is the two-dimensional concentration of scatterers.[2,5,11,12] Returns after two or more collisions [see Fig. 1(b)] give a smaller correction on the order of d/l.

In our previous work[13] we have drawn attention to another memory effect (the corridor effect) important in backscattering events. If a particle travels a distance x after which it is backscattered and returns to the initial point, the probability of this round trip of length $2x$ is proportional to $\exp(-x/l)$, not to $\exp(-2x/l)$, as would suggest the conventional Boltzmann approach, since the existence of a free corridor of width d allowing the first part of the journey guarantees a collisionless return. This effect also gives a correction to the diffusion coefficient on the order of d/l.

The role of memory effects becomes greatly enhanced in the presence of an applied magnetic field since the circling motion of an electron naturally increases the probability of returns, and many works were devoted to classical magnetoresistance, which for a degenerate 2D electron gas is entirely due to memory effects.[14] In particular, it was shown that the irreversibility introduced by the magnetic field destroys the corridor effect resulting in an anomalous magnetoresistance in classically weak magnetic fields.[13] An analytical theory of the anomalous low-field magnetoresistance was recently developed in Ref. 15.

The existing derivation[6,7] of the memory effect corrections is rather long and cumbersome being based on a special technique of the so-called ring diagrams. In the present paper we develop a relatively simple approach to the problem. We consider classical noninteracting particles with a fixed energy in two dimensions scattered by randomly positioned centers with a given differential cross section in the absence of magnetic field. We start with deriving a modified kinetic equation, which takes into account single returns after an

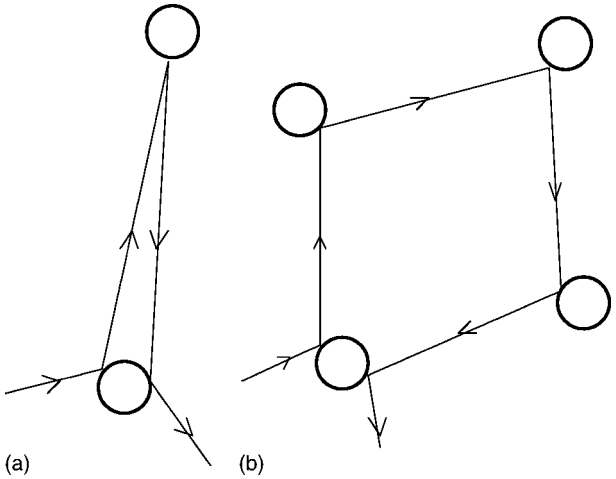

FIG. 1. Illustration of the memory effect due to return to the same scattering center after a single collision (a) or several collisions (b).

arbitrary number of collisions. We then derive the leading logarithmic correction to the diffusion coefficient for an arbitrary angular dependence of the differential cross section. Finally we find analytically the complete time dependence of the velocity correlation function for the special case of isotropic scattering taking into account the corridor effect and calculate the correction to the diffusion coefficient for this case. We perform numerical simulations for the cases of isotropic scattering and scattering by hard disks, and we find a good agreement between the numerical and analytical results.

II. DERIVATION OF THE BASIC EQUATION

The derivation of the conventional Boltzmann equation from the Liouville equation for a particle moving in the presence of randomly positioned scattering centers involves a number of simplifying assumptions. First, it is assumed that the mean free path l is much greater than the effective scattering diameter d or, otherwise that $Nd^2 \ll 1$, where N is the concentration of scatterers. Second, it is assumed that the distribution function does not change much on the space scale on the order of d and on the time scale on the order of d/v, where v is the modulus of the particle velocity, which is conserved since the scattering is elastic. These two conditions make it possible to describe scattering in terms of the differential cross section $\sigma(\phi)$ attributed to scattering centers positioned at given points in space. Third, memory effects are neglected: the Boltzmann approach is equivalent to randomly redistributing the scattering centers after each collision. Neglecting memory effects allows to take the average over the positions of scatterers in the Liouville equation, rather than use the average of its solution.

Restricting ourselves by the first two assumptions only, we can write down the following equation for the distribution function $f(\mathbf{r},\phi,t)$ (see Appendix A and Ref. 15 for the derivation of this equation in the simplest case of scattering by hard disks):

$$\frac{\partial f}{\partial t} + \mathbf{v}\frac{\partial f}{\partial \mathbf{r}} + v\sum_i \delta(\mathbf{r}-\mathbf{r}_i)\hat{T}f = 0, \tag{1}$$

where $\mathbf{r}_i$ are the coordinates of the scattering centers, and $\hat{T}$ is the scattering operator proportional to the Boltzmann collision integral

$$\hat{T}f = \int_0^{2\pi} \sigma(\phi-\phi')[f(\mathbf{r},\phi,t) - f(\mathbf{r},\phi',t)]d\phi'. \tag{2}$$

Note, that the distribution function f in Eq. (1) depends on the positions of scatterers $\mathbf{r}_i$ for a given realization. Also, since the scattering is elastic, the distribution function depends only on the polar angle ϕ of the velocity vector $\mathbf{v}$. The conventional Boltzmann equation can be obtained from Eq. (1) by replacing the actual density of scatterers $\Sigma_i\delta(\mathbf{r}-\mathbf{r}_i)$ by its average value N.

The correlation function $K(t)$ [normalized by the condition $K(0)=1$] and the diffusion coefficient D can be expressed through the solution of Eq. (1) with the following initial and normalization conditions:

$$f(\mathbf{r},\phi,0) = \delta(\mathbf{r})\delta(\phi), \qquad \int f(\mathbf{r},\phi,t)d\mathbf{r}d\phi = 1. \tag{3}$$

Then

$$K(t) = \int d\mathbf{r}\int_0^{2\pi} d\phi \cos\phi\langle f(\mathbf{r},\phi,t)\rangle, \tag{4}$$

$$D = \frac{v^2}{2}\int_0^{\infty} K(t)dt. \tag{5}$$

The angular brackets in Eq. (4) denote averaging over the positions $\mathbf{r}_i$ of the scattering centers.

We now develop a method to calculate $K(t)$ and D taking into account non-Boltzmann memory effects due to returns of the particle to previously visited scattering centers. As a first approximation we choose the solution $G(\mathbf{r}-\mathbf{r}',\phi,\phi',t)$ of the conventional Boltzmann equation

$$\frac{\partial G}{\partial t} + \mathbf{v}\frac{\partial G}{\partial \mathbf{r}} + vN\hat{T}G = 0 \tag{6}$$

with the initial condition

$$G(\mathbf{r}-\mathbf{r}',\phi,\phi',0) = \delta(\mathbf{r}-\mathbf{r}')\delta(\phi-\phi').$$

We rewrite Eq. (1) in the form

$$\frac{\partial f}{\partial t} + \mathbf{v}\frac{\partial f}{\partial \mathbf{r}} + Nv\hat{T}f = -\nu(\mathbf{r})\hat{T}f, \tag{7}$$

where $\nu(\mathbf{r}) = \Sigma_i\delta(\mathbf{r}-\mathbf{r}_i) - N$ is the fluctuation of the scatterer's concentration and $\langle\nu(\mathbf{r})\rangle = 0$. As above, the distribution function f in this equation depends on the actual positions of the scattering centers $\mathbf{r}_i$.

Equation (7) may be also written in an integral form using the formal solution of Eq. (6):

$$f(\mathbf{r},\phi,t) = G(\mathbf{r},\phi,0,t) - v\hat{G}\nu\hat{T}f, \tag{8}$$

where $\hat{G}$ is the integral operator with the kernel $G(\mathbf{r}-\mathbf{r}',\phi,\phi',t-t')$.

We now substitute f given by Eq. (8) into the right-hand side of Eq. (7) and we take the average of the resulting equation over the positions of the scatterers $\mathbf{r}_i$. In doing this we must deal with the product of functions $\nu(\mathbf{r})$, $\nu(\mathbf{r}')$, and the distribution function f, which all depend on the coordinates $\mathbf{r}_i$. We decouple f from the averaging procedure by writing

$$\langle\nu(\mathbf{r})\nu(\mathbf{r}')f\rangle \approx \langle\nu(\mathbf{r})\nu(\mathbf{r}')\rangle\langle f\rangle.$$

This approximation takes into account single returns to the same scattering center, but neglects multiple returns.

In the absence of correlation in the positions of the scatterers, which we assume to be true, we have

$$\langle\nu(\mathbf{r})\nu(\mathbf{r}')\rangle = N\delta(\mathbf{r}-\mathbf{r}').$$

Hence, we obtain the following equation for the averaged distribution function (to simplify the notations we replace hereafter $\langle f\rangle$ by f):

$$\frac{\partial f}{\partial t} + \mathbf{v}\frac{\partial f}{\partial \mathbf{r}} + Nv\hat{T}f = Nv^2 \int_0^{2\pi} d\phi' \int_0^t dt' \hat{T} G(0, \phi'' - \phi', t - t') \hat{T} f. \quad (9)$$

On the right-hand side of this equation the function $\hat{T}f$ is a function of ϕ', the left operator $\hat{T}$ acts on a function of the variable ϕ''.

The Green function $G(0, \phi'' - \phi', t)$ is the probability for a particle to return to the initial point after time t with velocity directed at angle ϕ'', provided that the initial velocity is directed at angle ϕ'. Obviously, this probability should depend on the difference $\phi'' - \phi'$ only [this is not the case for $G(\mathbf{r} - \mathbf{r}', \phi'', \phi', t)$ if $\mathbf{r} \neq \mathbf{r}'$].

The correction in the right-hand side of Eq. (9) coincides with the result of Weijland and Van Leeuwen[7] obtained by the ring-diagram technique. Equation (9) is the basis for the following calculations. The solution of this equation is needed for calculating the correlation function $K(t)$ and the diffusion coefficient D with the help of Eqs. (4) and (5). In fact, because of the approximations made during our derivation the right-hand side of this equation should be considered as a small perturbation.

III. DERIVATION OF THE CORRELATION FUNCTION AND THE DIFFUSION COEFFICIENT

To calculate $K(t)$ we need to know the integral of the distribution function over the coordinate

$$F(\phi, t) = \int f(\mathbf{r}, \phi, t) d\mathbf{r}. \quad (10)$$

Integrating Eq. (9) over $\mathbf{r}$ we get

$$\frac{dF}{dt} + Nv\hat{T}F = Nv^2 \int_0^{2\pi} d\phi' \int_0^t dt' \hat{T} G(0, \phi'' - \phi', t - t') \hat{T} F. \quad (11)$$

This equation can be further simplified by using the property that the functions $\exp(im\phi)$ are the eigenfunctions of the scattering operator $\hat{T}$:

$$Nv\hat{T}\exp(im\phi) = \gamma_m \exp(im\phi),$$

$$\gamma_m = Nv \int_0^{2\pi} [1 - \cos(m\phi)] \sigma(\phi) d\phi. \quad (12)$$

Expanding the functions F and G in Eq. (11) in Fourier series, we obtain

$$\frac{dF_m}{dt} + \gamma_m F_m = \frac{2\pi}{N} \gamma_m^2 \int_0^t dt' G_m(0, t - t') F_m(t'), \quad (13)$$

where

$$F_m(t) = \frac{1}{2\pi} \int_0^{2\pi} \exp(-im\phi) F(\phi, t) d\phi,$$

$$G_m(0, t) = \frac{1}{2\pi} \int_0^{2\pi} \exp(-im\phi) G(0, \phi, t) d\phi.$$

Equation (13) allows us to calculate any moment of the distribution function with the corrections due to returns taken into account.

As seen from Eqs. (4), (5), and (10), the correlation function and the diffusion coefficients can be expressed via the functions $F_1(t)$ and $F_{-1}(t) = F_1^*(t)$:

$$K(t) = 2\pi \,\mathrm{Re}\, F_1(t). \quad (14)$$

Equation (13) can be solved exactly. However, it should be noted that this equation, similar to our basic Eq. (9), takes into account single returns only and consequently gives the correct results only in the leading order in the small parameter Nd^2. For this reason, as we have already mentioned above, the right-hand term in Eq. (13) should be considered as a small perturbation. This means that in this term one can use the Boltzmann expression for $F_m(t)$:

$$F_m(t) = \frac{1}{2\pi} \exp(-\gamma_m t), \quad (15)$$

where the factor $(1/2\pi)$ appears because of the initial condition $F(\phi, 0) = \delta(\phi)$. Substituting this expression into the right-hand side of Eq. (13), for $m = 1$ we get

$$\frac{dF_1}{dt} + \gamma F_1 = \frac{\gamma^2}{N} \int_0^t G_1(0, t - t') \exp(-\gamma t') dt', \quad (16)$$

where

$$\gamma \equiv \gamma_1 = \tau^{-1} = Nv\sigma_{\mathrm{tr}} = Nv \int_0^{2\pi} \sigma(\phi)(1 - \cos\phi) d\phi$$

is the inverse momentum relaxation time, or transport time τ.

The solution of Eq. (16) can be easily found. After some manipulation it can be presented as follows:

$$F_1(t) = \frac{1}{2\pi} \exp(-\gamma t) + \frac{\gamma^2}{N} \int_0^t G_1(0, t - t') \exp(-\gamma t') t' dt'. \quad (17)$$

Finally, using Eq. (14) we obtain the following expression for the correlation function:

$$K(t) = K_0(t) + \delta K(t),$$

$$\delta K(t) = 2\pi \frac{\gamma^2}{N} \int_0^t G_1(0, t - t') \exp(-\gamma t') t' dt', \quad (18)$$

where $\delta K(t)$ is the correction to the Boltzmann result $K_0(t) = \exp(-\gamma t)$.

Substituting this expression into Eq. (5) and changing the order of integrations over t and t', we obtain a formula for the diffusion coefficient:

$$D = D_0 + \delta D, \quad D_0 = \frac{v^2}{2\gamma}, \quad \delta D = \frac{\pi v^2}{N} \int_0^\infty G_1(0, t) dt. \quad (19)$$

Here D_0 represents the Boltzmann result, while δD gives the correction due to returns, which is beyond the Boltzmann equation. One can see that calculation of these corrections is reduced to finding $G_1(0,t)$, which is equivalent to finding $G(0,\phi,t)$, the Boltzmann probability of return to the initial point $\mathbf{r}=0$ with velocity directed at angle ϕ with respect to the initial velocity.

IV. CONTRIBUTION OF RETURNS AFTER A SINGLE COLLISION

We have mentioned in the Introduction that the leading (logarithmic) correction to the diffusion coefficient is due to returns after a single collision (see Fig. 1). We will now show that the contribution of this process can be easily found for an arbitrary angular dependence of the scattering cross section $\sigma(\phi)$. To do this, we must find the corresponding contribution to the function $G(0,\phi,t)$.

We rewrite Eq. (6) in an integral form

$$G(\mathbf{r},\phi,t) = \delta(\mathbf{r}-\mathbf{v}_0 t)\,\delta(\phi)\exp(-\gamma_0 t) + Nv\int_0^{2\pi} d\phi'\,\sigma(\phi-\phi') \times \int_0^t \exp[-\gamma_0(t-t')]\,G[\mathbf{r}-\mathbf{v}'(t-t'),\phi',t']\,dt', \tag{20}$$

where $\gamma_0 = Nv\sigma$, σ is the total scattering cross section, $\mathbf{v}_0$ is the initial velocity (with $\phi=0$), and ϕ' is the angle of the vector $\mathbf{v}'$.

Equation (20) is convenient for obtaining the contribution of a given number of collisions before return by iterations. Since we are now interested in returns after a single collision, we can insert the zero approximation for G into the right-hand side of Eq. (20), equal to $\delta(\mathbf{r}-\mathbf{v}_0 t)\,\delta(\phi)\exp(-\gamma_0 t)$. Denoting the correction thus obtained as δG, we get

$$\delta G(\mathbf{r},\phi,t) = Nv\int_0^{2\pi} d\phi'\,\sigma(\phi-\phi')\int_0^t \exp[-\gamma_0(t-t')-\gamma_0 t'] \times \delta[\mathbf{r}-\mathbf{v}'(t-t')-\mathbf{v}_0 t']\,dt'. \tag{21}$$

Putting $\mathbf{r}=0$ and taking into account the relation

$$\delta[\mathbf{v}'(t-t')+\mathbf{v}_0 t'] = \frac{\delta(\phi'-\pi)}{v^2(t-t')}\,\delta(t-2t'),$$

we find

$$\delta G(0,\phi,t) = \frac{N}{v}\frac{\exp(-\gamma_0 t)}{t}\,\delta(\phi-\pi)\,\sigma(\phi). \tag{22}$$

Thus, for $\delta G_1(0,t)$ we obtain

$$\delta G_1(0,t) = -\frac{N}{2\pi v}\frac{\exp(-\gamma_0 t)}{t}\,\sigma(\pi). \tag{23a}$$

To find the correction δD to the diffusion coefficient we must substitute this expression in Eq. (19). The integral in Eq. (19) diverges logarithmically, which is the result of ignoring the finite radius of the scattering center. To avoid the divergence, we will replace t in the denominator of the expression Eq. (23a) by $t+t_0$, where the cutoff time t_0 is on the order of σ/v. Such a regularization seems reasonable, since it makes the return probability to be finite at $t\to 0$, as it should be if the finite radius of the scattering center is taken into account, and since our entire theory is applicable for time scales larger than σ/v.

Equation (23a) must be also corrected to include the corridor effect,[13,15] which we mentioned in the Introduction and which is not taken into account by Eq. (9). This effect is relevant for backscattering events, when the particle follows practically the same path (in the opposite direction) after a collision. The probability to make this round trip without collisions during time t should be $\exp(-\gamma_0 t/2)$ rather than $\exp(-\gamma_0 t)$ as Eq. (23a) says, because once the path $1\to 2$ during the time $t/2$ is collisionless, we are sure to have no collisions on the return path $2\to 1$. This effect can be taken into account by a more accurate evaluation of Eq. (1), which (within the approximation of pointlike scatterers) contains all memory effects, including the corridor effect, see Ref. 15 where this was done for scattering by hard disks. Here we will simply modify Eq. (23a) "by hand" replacing $\exp(-\gamma_0 t)$ by $\exp(-\gamma_0 t/2)$.

Thus, we replace Eq. (23a) by

$$\delta G_1(0,t) = -\frac{N}{2\pi v}\frac{\exp(-\gamma_0 t/2)}{t+t_0}\,\sigma(\pi). \tag{23b}$$

We then obtain the correction to the diffusion coefficient due to returns after a single collision

$$\frac{\delta D}{D_0} = N\sigma_{\mathrm{tr}}\sigma(\pi)\left[-\ln\left(\frac{1}{\gamma_0 t_0}\right)+\mathbf{C}-\ln 2\right], \tag{24}$$

where $D_0 = v^2/2\gamma$ is the Boltzmann value of the diffusion coefficient and $\mathbf{C}=0.577$ is the Euler constant. Since the exact numerical coefficient in the argument of the logarithm is unknown, the constant $\mathbf{C}-\ln 2$ could be safely discarded. We prefer to keep it in order to compare Eq. (24) with the more general formula derived in Sec. V and to have a clear definition of the cutoff parameter t_0 when discussing numerical results in Sec. VI.

With regard to this formula it should be noted that the argument of the logarithm contains the constant γ_0, which is expressed through the total scattering cross section. The latter is equal to infinity for any realistic scattering potential that does not drop to zero at a finite distance (as it is the case for scattering on hard disks when the total scattering diameter is of course equal to the disk diameter). The divergency of the total cross section is due to very small scattering angles. Since we consider the scattering centers as points, any scattering event will deviate the particle from its path connecting two scattering centers, however small the scattering angle may be. If the finite radius of the scatterer is taken into account, then scattering angles less than $\sim d/l$ will not matter anymore. This means that the integral over ϕ, which gives the total scattering cross section, entering the definition of γ_0, should in fact be truncated to exclude scattering angles

less than d/l. Because of the logarithmic dependence of δD on γ_0, the exact value, which should be attributed to this cutoff, is not very important.

Substituting Eq. (23b) into Eq. (18), we obtain the correction to the correlation function in the time interval $t_0 \ll t \ll \gamma_0^{-1}$:

$$\delta K(t) = -N\sigma_{\mathrm{tr}}\sigma(\pi)\gamma t \ln(t/t_0). \tag{25}$$

To conclude this section we note that returns after multiple collisions, which are important for times $t \gtrsim \tau$, give a correction to the diffusion coefficient on the order of $N\sigma_{\mathrm{tr}}^2$. Thus, as one can see from Eq. (24) the logarithmic correction dominates if $\sigma(\pi)$ is not too small, i.e., in all cases when the backscattering is not strongly suppressed.

V. CORRELATION FUNCTION FOR ISOTROPIC SCATTERING

For the special case of isotropic scattering $\sigma_{\mathrm{tr}}=\sigma$, $\sigma(\pi)=\sigma/2\pi$, and $\gamma_0=\gamma=\tau^{-1}=Nv\sigma$. This simplification allows to find analytically the Green function $G(0,\phi,t)$ for arbitrary times (that are larger than the cutoff time t_0).

The details of the calculation are given in Appendix B. The function $G_1(0,t)$, through which the corrections to the correlation function and the diffusion coefficient are expressed, has the form

$$G_1(0,t) = \frac{\gamma^2}{4\pi^2 v^2}\left(-\frac{\exp(-x/2)}{x+x_0} + \frac{1-\exp(-x)}{x} + 2\exp(-x)[\mathrm{Ei}(x) - \mathrm{Ei}(2x)]\right), \tag{26}$$

where we have introduced the notations $x=t/\tau$, $x_0=t_0/\tau \ll 1$, and $\mathrm{Ei}(x)=-\int_{-x}^{\infty} dy \exp(-y)/y$ is the integral exponent. Since $t_0 \sim \sigma/v$ and $\tau=(N\sigma v)^{-1}$, the cutoff parameter can be presented as $x_0=\alpha N\sigma^2$, where α is an unknown constant on the order of unity.

Comparing Eqs. (26) and (23b), one can see that the first term in Eq. (26) represents the contribution from returns after a single collision with the cutoff at $t \to 0$ and the corridor effect taken into account as described in the previous section. The other terms in Eq. (26) correspond to returns after two or more collisions and do not contain any singularities.

A direct calculation using Eqs. (19) and (26) gives us the correction to the diffusion coefficient

$$\frac{\delta D}{D_0} = \frac{N\sigma^2}{2\pi}\left[-\ln\left(\frac{1}{x_0}\right) + \mathbf{C} - 2\ln 2\right] \tag{27}$$

which differs from Eq. (24) describing the contribution of returns after a single collision by an additional term $(-\ln 2)$ in the brackets, which is the contribution of returns after multiple collisions.

The correction to the correlation function, $\delta K(t)$ can now be calculated by using the Eqs. (26) and (18). A direct calculation gives the following, rather cumbersome, expression (here again $x=t/\tau$):

$$\delta K(t) = -\frac{N\sigma^2}{2\pi}\kappa(x),$$

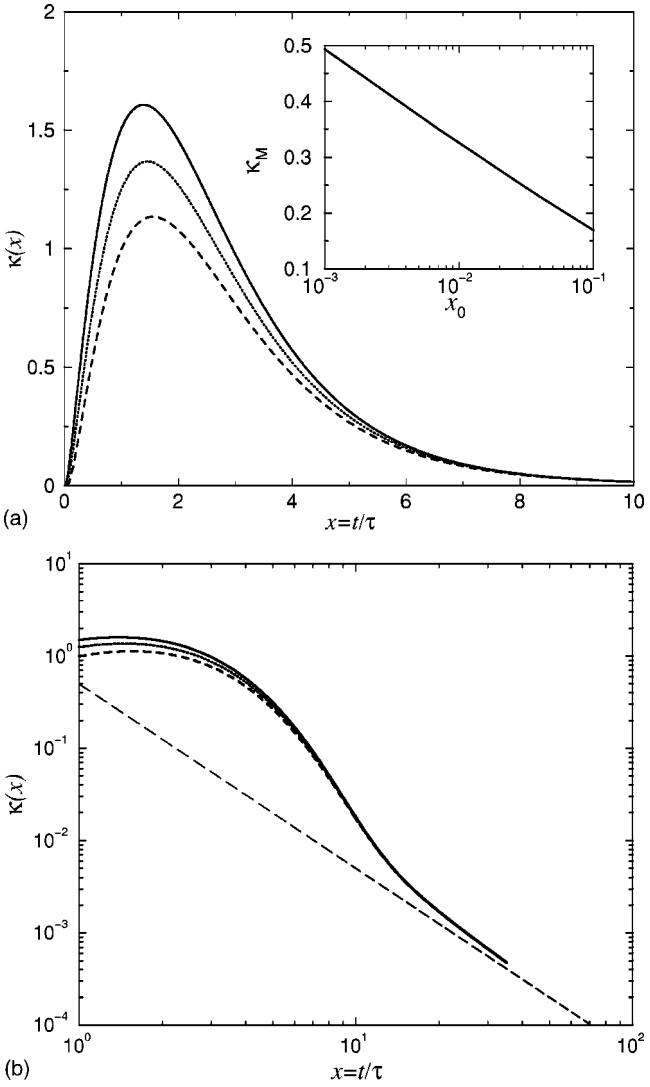

FIG. 2. (a) Plot of $\kappa(x)=-(2\pi/N\sigma^2)\delta K(x)$ versus $x=t/\tau$ for different values of the cutoff parameter x_0. Continuous, dotted, and dashed curves correspond to $x_0=0.01$, 0.02, and 0.04, respectively. The inset shows the dependence of the maximum value κ_M on $\ln x_0$. (b) The long time part is emphasized in a log-log plot to show that the different curves become quickly superimposed for $x>5$ and reach very slowly the asymptotic regime, $1/2x^2$, as $x \to \infty$ (shown by the long-dashed line).

$$\kappa(x) = 3e^{-x} - 2e^{-x/2} - 1 + 2e^{-2x}[\mathrm{Ei}(2x) - \mathrm{Ei}(x)] + (x+x_0)e^{-x}\left[\mathrm{Ei}\left(\frac{x+x_0}{2}\right) - \mathrm{Ei}\left(\frac{x_0}{2}\right)\right] + e^{-x}\{(x-2)[\mathrm{Ei}(x) - \mathbf{C} - \ln x] + x + 2(x-1)\ln 2\}. \tag{28}$$

The function $\kappa(x)$ is presented in Fig. 2(a) for several values of the cutoff parameter x_0. In inset is shown the linear dependence of the maximum value of $\kappa(x)$ on $\ln x_0$.

For small times, $x_0 \ll x \ll 1$, Eq. (28) gives

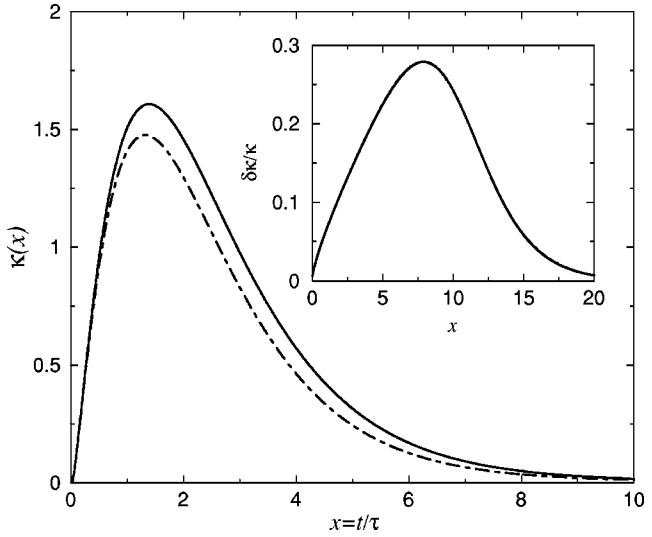

FIG. 3. Plot of $\kappa(x)$ (continuous line) and $\tilde{\kappa}(x)$ (dot-dashed line), given by Eqs. (28) and (B8), respectively, for the same value of the cutoff parameter $x_0=0.01$. The relative difference $(\kappa-\tilde{\kappa})/\kappa$ is shown in the inset.

$$\kappa(x) = x\,\ln(x/x_0), \tag{29}$$

so that $\delta K(t)$ coincides with the expression given by Eq. (25), if one takes into account that for isotropic scattering $\sigma_{tr}=\sigma$ and $\sigma(\pi)=\sigma/2\pi$. At large times, $x\gg 1$, the correlation function is dominated by the contribution of returns over long diffusive trajectories involving many collisions. It can be presented as a series in inverse powers of t. Using Eq. (28) in this limit, we obtain the leading terms of this expansion

$$\kappa(x) = \frac{1}{2x^2}\left(1+\frac{5}{x}\right). \tag{30}$$

The leading term ($\sim 1/t^2$) coincides with the known result obtained by Ernst and Weyland,[9] while the second one gives the first correction. We note that the leading term (but not the correction) is a universal result, which can be derived in the diffusion approximation[9] and which does not depend on the scattering cross-section. It can be seen that the asymptotic $1/t^2$ behavior is approached very slowly, so that even for $t=50\tau$ ($x=50$) the correction still makes 10% [see Fig. 2(b)]. This explains why the predicted asymptotic behavior was not reached in the numerical simulations done by Bruin,[10] as well as in our simulations to be presented in the next section.

Finally, in Fig. 3, we present, for comparison, the function $\tilde{\kappa}(x)$ given in Appendix B, Eq. (B8), in which the corridor effect is not taken into account. One can see that the role of the corridor effect is noticeable, but rather small.

VI. NUMERICAL SIMULATIONS

Using a random number generator, the centers of $\mathcal{N}$ disks of diameter d are uniformly randomly positioned on a plane inside a square box of edge length L. We take $L/d=1000$ to be sure that L remains more than one order of magnitude larger than the mean free path, even for the smallest concentrations that we have considered. The value of $\mathcal{N}$ is chosen to obtain the desired value for the dimensionless concentration, $\mathcal{N}d^2/L^2=Nd^2$. Numerical simulations were performed for Nd^2 equal to 0.064, 0.032, and 0.016. To calculate the velocity correlation function $K(t)$, as well as the diffusion coefficient D given by Eq. (5), we first choose an initial point at random inside the box with an initial velocity direction arbitrarily chosen along the x direction. We then determine the trajectory of a pointlike particle by joining the successive impact points, an impact point being the first intersection, calculated analytically, of the linear trajectory with a disk periphery, the particle always coming from outside of the disk. We use standard numerical tricks to accelerate the search for impacts. When choosing the initial position, the disk interiors are not excluded (it was checked that excluding them introduces only a weak numerical difference, which vanishes in the limit $Nd^2\to 0$). The trajectory is made of successive straightline segments between collisions. Periodic boundary conditions are imposed at the edges of the square box.

In the hard-disk (or Lorentz) model the scattering angle ϕ is related to the impact parameter ρ by $\rho=(d/2)\cos(\phi/2)$ (we consider $0<\phi<2\pi$, so that ρ may be negative). The differential cross section $\sigma(\phi)=|d\rho/d\phi|=(d/4)\sin(\phi/2)$ is anisotropic, with enhanced backscattering (in contrast to isotropic scattering by hard spheres in three dimensions). As a consequence, the transport cross section is larger than the total cross section: $\sigma_{tr}=(4/3)d$.

To simulate isotropic scattering we define the scattering angle by the relation $\rho=(d/2)(1-\phi/\pi)$, so that $\sigma(\phi)=d/2\pi$. This relation is somewhat artificial, it leads to unrealistic situations, in which the disk may be cut by the scattering trajectory. This isotropic model, which is built to have an angle-independent differential scattering cross section, does not correspond to any realistic potential and is considered for the sole purpose to check our analytical theory.

In order to calculate the correlation function $K(x)$ and its dimensionless integral up to a time $t=x\tau$, $I(t)=\int_0^{t/\tau}K(x)dx=X(t)/v\tau$, where $X(t)$ is the overall displacement of the particle in the x direction during time t, we consider a set of 5000 discrete values x_n of the reduced time $x=t/\tau$, regularly spaced up to $x_m=20$, and we calculate both quantities for each x_n. The values of $K(x_n)$ and $I(x_n)$ are averaged over 100 disk configurations and 10^8 trials for the starting point, except for the lowest concentration $Nd^2=0.016$ where only 10^7 trials for the starting point were considered. In this way we get practically continuous curves for both $K(t)$ and $I(t)$. The reduced value of the diffusion coefficient D/D_0 is obtained by extrapolation of the results for $I(t)$ to $t\to\infty$.

In Fig. 4, we present the numerical results for $K(t)$ for the isotropic scattering together with the pure exponential curve $K_0(t)=e^{-t/\tau}$ expected from the Boltzmann approach. The enlarged scale in Fig. 4(b) allows us to clearly see the negative departure from the exponential behavior and the long-time tail of the correlation function. We have also calculated numerically the correlation function for the hard disk scattering. The results are qualitatively similar to the isotropic case and agree with the numerical simulations of Bruin.[10]

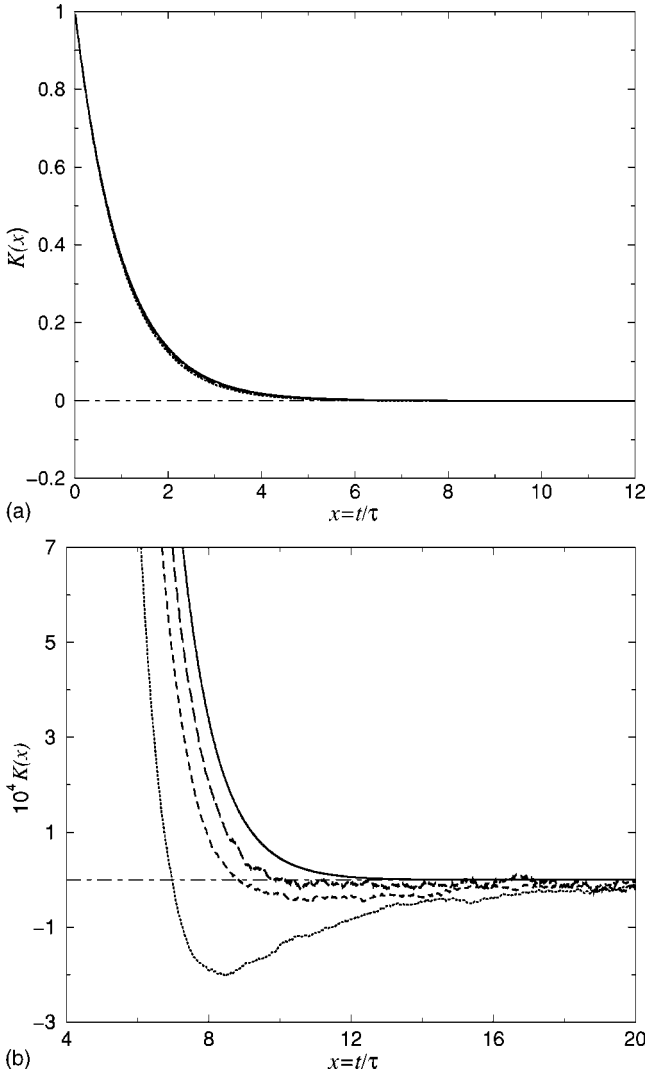

FIG. 4. (a) Results of the numerical calculations for the isotropic model as a plot of $K(x)$ for different concentrations. Dotted, dashed, and long-dashed curves correspond to $Nd^2=0.064$, 0.032, and 0.016, respectively. The pure exponential $K_0=\exp(-x)$ is shown by the continuous curve. (b) For $t>4\tau$ the scale is enlarged by a factor 10^4 to better show the difference between $K(x)$ and $K_0(x)$.

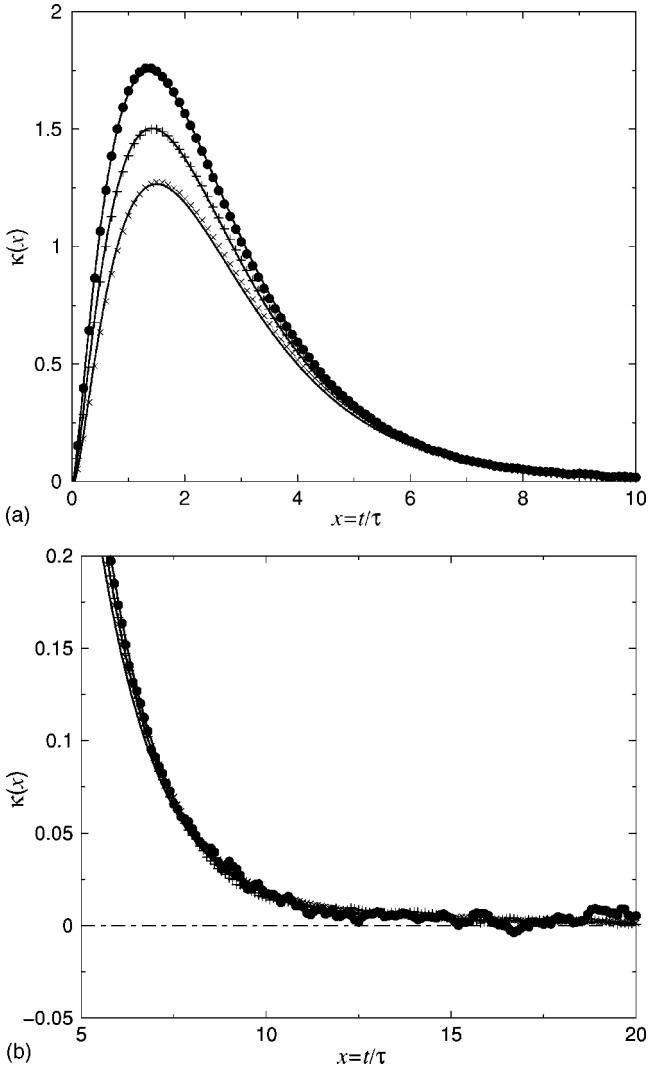

FIG. 5. (a) The results of the preceding figures are reported in a plot of $\kappa(x)$. Only 200 points are selected in the range $0<x<20$. Crosses, plus signs, and filled circles correspond to $Nd^2=0.064$, 0.032, and 0.016, respectively. The continuous lines correspond to the fits obtained using Eq. (28) with the same proportionality factor. $\alpha=0.424$, between x_0 and Nd^2 in the three cases. The error bars are smaller than the symbol size. (b) The region $x>5$ is shown with a larger scale. At this new scale one can see the fluctuations of the numerical data giving an idea of the magnitude of the error bars (which are larger in the case $Nd^2=0.016$ due to the poorer statistics).

Figure 5 presents the comparison of the numerical results for the normalized correction to the correlation function $\kappa(x)$ for isotropic scattering with the theoretical formula given by Eq. (28). The only fitting parameter is the constant α in the definition of the cutoff value of $x_0=\alpha Nd^2$. By choosing $\alpha=0.424$ we obtain a practically perfect fit to the theoretical curves for several values of Nd^2. The numerical errors are responsible for the noisy character of the simulation data for $x>10$, however they are practically negligible for smaller values of x, the error bar being smaller than the symbol size.

Because of the high precision of our numerical simulation, we are able to verify the theoretical prediction concerning the role of the corridor effect. For this purpose we try to fit the numerical data to the function $\tilde{\kappa}(x)$ given by Eq. (B8), which does not take care of this effect, see Fig. 6. It is not possible to have a good fit with the same choice of the constant α as before. Thus we chose a different value, $\alpha=0.283$, to fit the maxima of the numerical curves. As it can be seen from Fig. 5, though the resulting fit could be considered as satisfactory, the difference is well beyond the numerical errors, in particular the numerical data points for $5<x<10$ are systematically above the theoretical curves. Comparing Figs. 5 and 6, one can see that taking the corridor effect into account makes the agreement between the theoretical and numerical curves substantially better.

Finally, in Fig. 7 we present the numerical results for the correction to the diffusion coefficient $\delta D/D_0$ in units of $Nd^2/2\pi$ versus $\ln(1/Nd^2)$, see Eq. (27). Data for both the hard-disk scattering and isotropic scattering are presented for

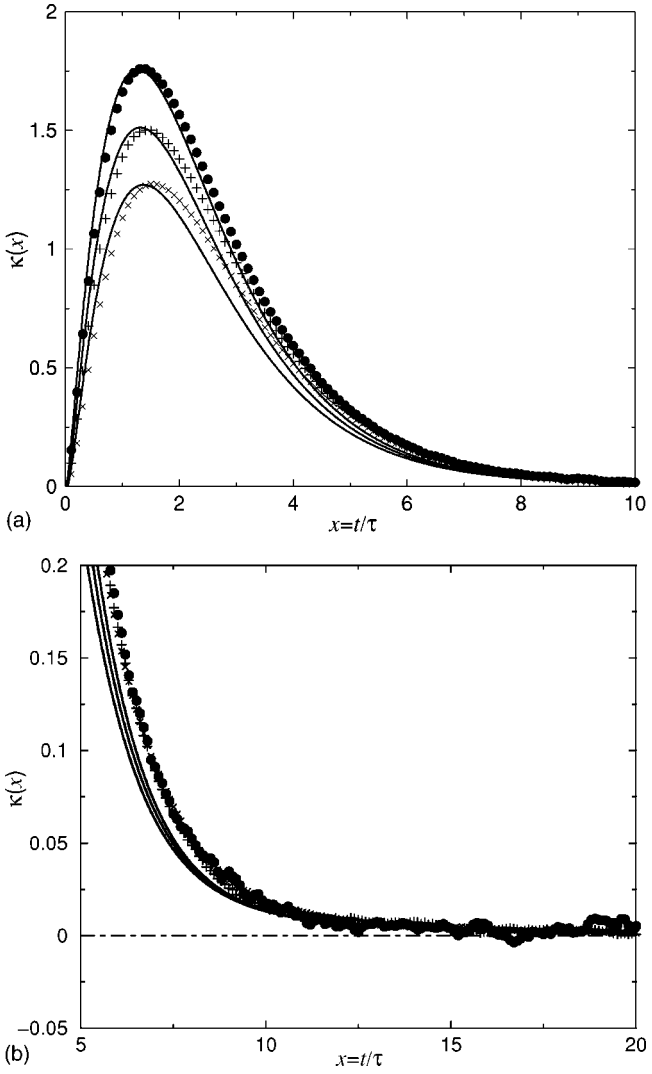

FIG. 6. (a) The same numerical results are fitted by Eq. (B8), which does not take care of the corridor effect. Here, to fit the maximum values, we take a different proportionality factor than in Fig. 5, namely, $\alpha=0.283$. (b) The region $x>5$ is shown with a larger scale.

several values of Nd^2. For the case of isotropic scattering we get an excellent agreement with Eq. (27), in which the cutoff parameter is chosen as in Fig. 4: $x_0=0.424Nd^2$. The slope of the dependence on $\ln(1/Nd^2)$ in the general case is given by Eq. (24). For the hard-disk scattering the slope is equal to 1.95 ± 0.10, which is close to what follows from Eq. (24). Indeed, for a given diameter d, the ratio of $\sigma_{\mathrm{tr}}\sigma(\pi)$ for the two cases is equal to $2\pi/3=2.094$.

VII. CONCLUSION

In this paper, we have presented a simple approach to the problem of classical corrections to the Boltzmann equation, which are due to memory effects. We have performed both analytical and numerical calculations of the velocity autocorrelation function for noninteracting particles scattered by randomly located centers in two dimensions.

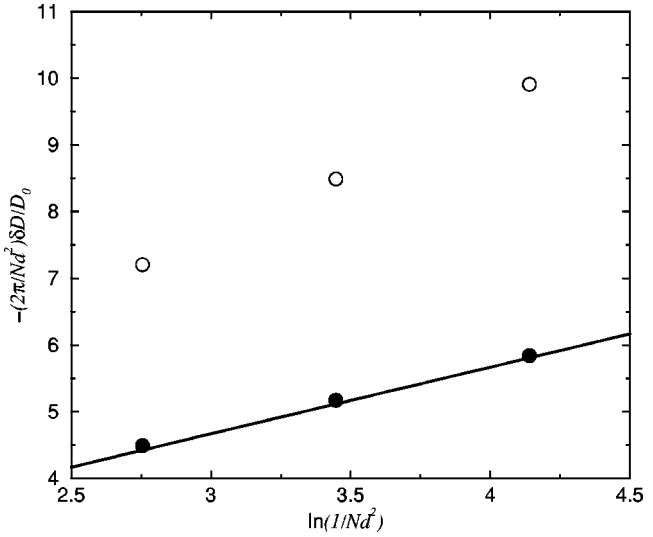

FIG. 7. Numerical results for the diffusion coefficient as a plot of $-(2\pi/Nd^2)\delta D/D_0$ versus $\ln(1/Nd^2)$ for the hard disk scattering (open circles) and for isotropic scattering (filled circles). The linear behavior predicted by formula (27) in the isotropic case, with $\alpha=0.424$ as in Fig. 5, is represented by the straight line (of slope 1). A linear fit through the three points in the hard disk case gives a slope of 1.95 ± 0.10 in good agreement with the theoretical prediction of 2.094.

In the particular case of isotropic scattering, we were able to provide a full analytical expression for the correction to the Boltzmann result, due to returns of the particles to previously visited regions, in excellent agreement with the results of numerical simulations. Furthermore, the comparison between analytical and numerical results demonstrates that it is essential to take care of the "corridor effect" associated with backscattering events. In the case of hard disk scattering (Lorentz model), we obtain a good agreement for the dependence of the diffusion coefficient on the concentration of scattering centers. A full theory taking into account both classical and quantum (weak localization) memory effects is needed to understand the relative role of classical and quantum corrections depending on the ratio of the De Broglie wavelength to the scattering diameter.

ACKNOWLEDGMENTS

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APPENDIX A

For the case of scattering by hard disks, the Liouville equation has the form[6,7,15]

$$\frac{\partial f}{\partial t}+\mathbf{v}\frac{\partial f}{\partial \mathbf{r}}+v(\hat{T}_-+\hat{T}_+)f=0, \tag{A1}$$

where the operators $\hat{T}_-$ and $\hat{T}_+$ describe scattering by the disks. They are defined by the equations

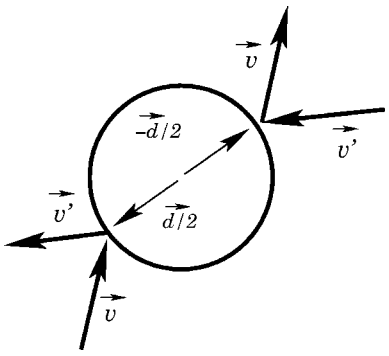

FIG. 8. Scattering of a particle by a hard disk. Scattering events described by the operators T_- and T_+ are shown.

$$\hat{T}_- f(\mathbf{r},\phi,t) = \sum_i \int_0^{2\pi} d\phi'\, \delta(\mathbf{r} - \mathbf{r}_i - \mathbf{d}/2)\sigma(\phi - \phi') f(\mathbf{r},\phi,t), \tag{A2}$$

$$\hat{T}_+ f(\mathbf{r},\phi,t) = -\sum_i \int_0^{2\pi} d\phi'\, \delta(\mathbf{r} - \mathbf{r}_i + \mathbf{d}/2)\sigma(\phi - \phi') f(\mathbf{r},\phi',t). \tag{A3}$$

Here $\sigma(\phi) = (d/4)\sin(\phi/2)$ is the differential cross section for a disk of diameter d, the vector $\mathbf{d}$ is expressed through the velocities before and after the collision, $\mathbf{v}$ and $\mathbf{v}'$ by the relation (see Fig. 8)

$$\mathbf{d} = d\frac{\mathbf{v}' - \mathbf{v}}{\sqrt{2(v^2 - \mathbf{v}\cdot\mathbf{v}')}}. \tag{A4}$$

Equation (A1) is exact, the operators $\hat{T}_-$ and $\hat{T}_+$ describing the mechanics of collisions (assuming that the disks do not overlap). The term $\hat{T}_- f$ describes the outflux of particles from the state with velocity $\mathbf{v}$ at the point $\mathbf{r}_i + \mathbf{d}/2$ on the disk edge, while the term $\hat{T}_+ f$ describes the influx of particles to the state with velocity $\mathbf{v}$ at the point $\mathbf{r}_i - \mathbf{d}/2$ (see Fig. 8).

If we make the assumption that the distribution function $f(\mathbf{r},\phi,t)$ can be regarded as constant on distances on the order of d, we can neglect the vector $\mathbf{d}/2$ in the arguments of the δ functions in Eqs. (A2) and (A3). Then we immediately obtain Eq. (1).

APPENDIX B

For the case of isotropic scattering, we write the Boltzmann equation for the function G in the form

$$\frac{\partial G}{\partial t} + \mathbf{v}\frac{\partial G}{\partial \mathbf{r}} + \gamma(G - G_0) = \delta(\mathbf{r})\delta(\phi)\delta(t), \tag{B1}$$

where

$$G_0(\mathbf{r},t) = \frac{1}{2\pi}\int_0^{2\pi} G(\mathbf{r},\phi,t)d\phi$$

is the isotropic part of $G(\mathbf{r},\phi,t)$. Performing the Fourier transformation of this equation in variables $\mathbf{r}$ and t, we obtain

$$-i(\omega - \mathbf{k}\cdot\mathbf{v})G(\mathbf{k},\phi,\omega) + \gamma[G(\mathbf{k},\phi,\omega) - G_0(\mathbf{k},\omega)] = \delta(\phi). \tag{B2}$$

If we find $G(\mathbf{k},\phi,\omega)$ from this equation and take its average over the angle ϕ, we will have an algebraic equation for $G_0(\mathbf{k},\omega)$. Solving it and using Eq. (B2), we obtain the following expression for the function $G(\mathbf{k},\phi,\omega)$:

$$G(\mathbf{k},\phi,\omega) = \frac{\delta(\phi)}{\gamma - i\omega + ikv\cos\phi_k} + \frac{\gamma g(k,\omega)}{2\pi[\gamma - i\omega + ikv\cos(\phi - \phi_k)](\gamma - i\omega + ikv\cos\phi_k)[g(k,\omega) - \gamma]}, \tag{B3}$$

where ϕ_k is the angle of the vector $\mathbf{k}$ and $g(k,\omega) = \sqrt{(\gamma - i\omega)^2 + k^2v^2}$.

Now we can easily find the expression for $G_1(\mathbf{k},\omega)$:

$$G_1(\mathbf{k},\omega) = \frac{1}{2\pi(\gamma - i\omega + ikv\cos\phi_k)} + \frac{\gamma\exp(-i\phi_k)}{2\pi ikv}\frac{g(k,\omega) - \gamma + i\omega}{(\gamma - i\omega + ikv\cos\phi_k)[g(k,\omega) - \gamma]}. \tag{B4}$$

The function $G_1(0,t)$ entering Eqs. (18) and (19) is given by the Fourier transform of Eq. (B4) for $\mathbf{r} = 0$. The first term in Eq. (B4) then becomes $\exp(-\gamma t)\delta(\mathbf{v}_0 t)$. This contribution should be omited, since it does not describe returns for $t > 0$. We begin the Fourier transformation of the second term by calculating the integral over the angle ϕ_k using the formula[16]

$$\int_{-\pi}^{\pi}\frac{\exp(-i\phi)}{1 + a\cos\phi}d\phi = 2\int_0^{\pi}\frac{\cos\phi}{1 + a\cos\phi}d\phi = \frac{2\pi}{a}\frac{\sqrt{1 - a^2} - 1}{\sqrt{1 - a^2}}.$$

Then we have

$$G_1(0,t) = -\frac{\gamma}{(2\pi)^2 v^2}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}e^{-i\omega t}\int_0^{\infty}\frac{dk}{k}\frac{[g(k,\omega) - \gamma + i\omega]^2}{g(k,\omega)[g(k,\omega) - \gamma]}. \tag{B5}$$

Instead of k we now introduce a new variable $z = g(k,\omega) - \gamma + i\omega$, which gives us

$$G_1(0,t) = -\frac{\gamma}{(2\pi)^2 v^2}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}e^{-i\omega t}\int_0^{\infty}\frac{zdz}{[z+2(\gamma-i\omega)](z-i\omega)}. \tag{B6}$$

The integral over ω can be now easily calculated and the remaining integral over z gives

$$G_1(0,t) = \frac{\gamma^2}{4\pi^2 v^2}\left(-\frac{\exp(-x)}{x}+\frac{1-\exp(-x)}{x} + 2\exp(-x)[\mathrm{Ei}(x)-\mathrm{Ei}(2x)]\right), \tag{B7}$$

where $x=\gamma t$. After replacing $\exp(-x)$ by $\exp(-x/2)$ in the first term to account for the corridor effect and introducing the cutoff at $t_0=x_0/\gamma$ as described in Sec. IV, we obtain Eq. (26).

If we neglect the corridor effect (but still introduce the cutoff at t_0), Eq. (B7) can be used directly to calculate the correction to the correlation function. Inserting Eq. (B7) into Eq. (18) we get, instead of $\kappa(x)$ given by Eq. (28), the following expression for $\tilde{\kappa}(x)$, which does not take into account the corridor effect:

$$\tilde{\kappa}(x) = -1+2e^{-2x}[\mathrm{Ei}(2x)-\mathrm{Ei}(x)]+e^{-x}\left[1+(x-2)[\mathrm{Ei}(x) - \mathbf{C} - \ln x] + 2(x-1)\ln 2 + (x+x_0)\ln\left(1+\frac{x}{x_0}\right)\right]. \tag{B8}$$

[1] J. R. Dorfman and E. G. D. Cohen, Phys. Lett. **16**, 124 (1965).
[2] J. V. Sengers, Phys. Rev. Lett. **15**, 515 (1965).
[3] K. Kawasaki and I. Oppenheim, Phys. Rev. **139A**, 1763 (1965).
[4] J. Weinstock, Phys. Rev. **140**, A460 (1965).
[5] L. K. Haines, J. R. Dorfman, and M. H. Ernst, Phys. Rev. **144**, 207 (1966).
[6] J. M. J. Van Leeuwen and A. Weijland, Physica (Amsterdam) **36**, 457 (1967).
[7] A. Weijland and J. M. J. Van Leeuwen, Physica (Amsterdam) **38**, 35 (1968).
[8] B. J. Alder and T. E. Wainwright, Phys. Rev. A **1**, 18 (1970).
[9] M. H. Ernst and A. Weyland, Phys. Lett. **34A**, 39 (1971).
[10] C. Bruin, Phys. Rev. Lett. **29**, 1670 (1972).
[11] R. Peierls, *Surprises in Theoretical Physics* (Princeton University Press, Princeton, 1979).
[12] E. H. Hauge, in *Transport Phenomena*, edited by G. Kirczenov and J. Marro, Lecture Notes in Physics No. 31 (Springer, New York, 1974), p. 337.
[13] A. Dmitriev, M. Dyakonov, and R. Jullien, Phys. Rev. Lett. **89**, 266804 (2002).
[14] E. M. Baskin, L. N. Magarill, and M. V. Entin, Sov. Phys. JETP **48**, 365 (1978); D. Polyakov, *ibid.* **63**, 317 (1986); A. V. Bobylev, F. A. Maaø, A. Hansen, and E. H. Hauge, Phys. Rev. Lett. **75**, 197 (1995); A. V. Bobylev, F. A. Maaø, A. Hansen, and E. H. Hauge, J. Stat. Phys. **87**, 1205 (1997); E. M. Baskin and M. V. Entin, Physica B **249-251**, 805 (1998); M. M. Fogler, A. Yu. Dobin, V. I. Perel, and B. I. Shklovskii, Phys. Rev. B **56**, 6823 (1997); A. D. Mirlin, J. Wilke, F. Evers, D. G. Polyakov, and P. Wolfle, Phys. Rev. Lett. **83**, 2801 (1999); A. D. Mirlin, D. G. Polyakov, F. Evers, and P. Wolfle, *ibid.* **87**, 126805 (2001); A. Dmitriev, M. Dyakonov, and R. Jullien, Phys. Rev. B **64**, 233321 (2001).
[15] V. Cheianov, A. P. Dmitriev, and V. Yu. Kachorovskii, Phys. Rev. B **68**, 201304(R) (2003).
[16] I. S. Gradshtei'n and I. M. Ryzhik, *Table of Integrals, Series, and Products* (Academic, New York, 1980), p. 366.