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KINETIC THEORY OF SELF-DIFFUSION IN A MODERATELY DENSE ONE-COMPONENT PLASMA

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A microscopic description of self-diffusion in a moderately dense classical one-component plasma is given on the basis of renormalized kinetic theory. The effects of close binary collisions and of collective interactions in the plasma are taken into account through the use of a composite memory kernel that includes both the Boltzmann and the Balescu–Guernsey–Lenard kernels as special cases. The composite kernel satisfies the lowest-order sum rule by virtue of the approximate validity of the hypernetted-chain equation for the static plasma correlation function. The ensuing values of the self-diffusion coefficient are obtained numerically for several plasma densities and are compared with the results of previous theories and of molecular dynamics.

1. Introduction

The evaluation of transport coefficients for a dilute plasma by means of kinetic equations often leads to divergent results[1]). The reason for the occurrence of these infinities is that in a plasma both close binary collisions and collective interactions play an essential role in the transport phenomena. In the kinetic equations of Balescu–Guernsey–Lenard and Boltzmann either the former or the latter processes are neglected; Landau's equation is a hybrid of the other two and has the deficiencies of both of them. Frequently a cutoff has been used to render the kinetic expressions for the transport coefficients finite. In a more systematic approach the various interactions in the plasma are taken into account by starting from a kinetic equation with a composite collision term that is a unification of those of the Balescu–Guernsey–Lenard and the Boltzmann equations; the finiteness of the transport coefficients is then guaranteed from the beginning[2–4]).

In the last few years the transport properties of plasmas with higher densities have been studied with the help of the methods of liquid kinetic theory[5]). Instead of the one-particle distribution functions that constitute the central quantities in the older kinetic theories attention is focused on the time correlation functions from which the transport coefficients follow by means of Green–Kubo relations. Dressing effects in the plasma are included by 'renormalizing' the interparticle potential that governs the evolution of the

time correlation function. Under suitable approximations the memory kernel of the kinetic equation for the correlation function then reduces to a generalized form of the Balescu–Guernsey–Lenard kernel[6,7]). Although this generalized kernel has the virtue of yielding convergent expressions for the transport coefficients, it gives an incomplete description of the underlying processes since close collisions in the plasma are treated incorrectly.

In the present paper it will be demonstrated how close collisions in the plasma can be incorporated in the formalism by introducing a memory kernel that is a generalization of the composite kernel of dilute-plasma theory. In particular, we shall consider the self-diffusion process that refers to the motion of a tagged particle. As a model we shall take the classical one-component plasma that consists of a system of charged particles in an inert uniform background of opposite charge.

In section 2 the general formalism of renormalized kinetic theory will be introduced. As a starting point for the discussion of dense plasmas we shall adopt the second-order mean-field approximation of the memory kernel for the self-diffusion time correlation function. In the next section it will be shown how this mean-field kernel reduces to generalized forms of the well-known memory kernels of standard dilute-plasma kinetic theory. After a discussion of the general properties of the various kernels in section 4 a composite kernel that describes both close and remote plasma interactions will be introduced in section 5. In the last section numerical values of the self-diffusion coefficient will be obtained for plasmas of moderate density.

2. Renormalized kinetic theory

The motion of a tagged particle through a fluid in equilibrium may be described in terms of time correlation functions, the simplest of which is defined as

$$C^s(\boldsymbol{r}\boldsymbol{p};\boldsymbol{r}'\boldsymbol{p}';t) = \langle \delta f^s(\boldsymbol{r}\boldsymbol{p};t)\delta f^s(\boldsymbol{r}'\boldsymbol{p}';0)\rangle. \tag{1}$$

The phase function f^s appearing inside the canonical-ensemble average is a product of delta functions fixing the position $\boldsymbol{r}_s(t)$ and momentum $\boldsymbol{p}_s(t)$ of the tagged particle:

$$f^s(\boldsymbol{r}\boldsymbol{p};t) = \sqrt{N}\,\delta[\boldsymbol{r} - \boldsymbol{r}_s(t)]\delta[\boldsymbol{p} - \boldsymbol{p}_s(t)], \tag{2}$$

with N the total number of particles in the fluid system; furthermore the symbol δ in (1) denotes the deviation from the equilibrium value, so that $\delta f^s = f^s - \langle f^s\rangle = f^s - (n/\sqrt{N})f_0(p)$, with n the particle density and $f_0(p)$ the normalized Maxwell–Boltzmann distribution function. More general tagged-

particle time correlation functions $C^s_{k,l}$, which for $k = l = 1$ reduce to C^s, are introduced by writing

$$C^s_{k,l}(r_1p_1 \ldots r_kp_k\,; r'_1p'_1 \ldots r'_lp'_l\,; t)$$
$$= \langle \delta[f^s(r_1p_1\,; t)f(r_2p_2\,; t) \ldots f(r_kp_k\,; t)]$$
$$\delta[f^s(r'_1p'_1\,; t)f(r'_2p'_2\,; t) \ldots f(r'_lp'_l\,; t)]\rangle, \tag{3}$$

with phase functions f given by

$$f(rp\,; t) = \sum_{i=1}^{N} \delta[r - r_i(t)]\delta[p - p_i(t)]. \tag{4}$$

The time correlation functions $C_{k,l}$ for arbitrary particles in the fluid have the same form as (3), with f^s replaced by f. The static correlation functions obtained by putting $t = 0$ will be denoted by $\tilde{C}^s_{k,l}$ and $\tilde{C}_{k,l}$; for $k = l = 1$ one finds in particular

$$\tilde{C}^s(rp\,; r'p') = nf_0(p)\delta(r - r')\delta(p - p'), \tag{5}$$

$$\tilde{C}(rp\,; r'p') = nf_0(p)\delta(r - r')\delta(p - p') + n^2f_0(p)f_0(p')h(r - r'), \tag{6}$$

with $h(r) = g(r) - 1$ the pair correlation function.

The self-diffusion coefficient D can be found directly from C^s; in fact, upon introducing the Laplace transform

$$C^s(rp\,; r'p'\,; z) = -\mathrm{i}\int_0^\infty \mathrm{d}t\, \mathrm{e}^{\mathrm{i}zt}C^s(rp\,; r'p'\,; t), \tag{7}$$

with $\mathrm{Im}\, z > 0$, one may write the Green–Kubo relation in the form

$$D = \mathrm{i}/(3m^2n) \lim_{z \to \mathrm{i}0} V^{-1} \int \mathrm{d}r\, \mathrm{d}r'\, \mathrm{d}p\, \mathrm{d}p'\, p \cdot p' C^s(rp\,; r'p'\,; z). \tag{8}$$

The time correlation function $C^s(z)$ will satisfy a kinetic equation of the general form

$$[z - L_0(rp)]C^s(rp\,; r'p'\,; z)$$
$$- \int \mathrm{d}r''\, \mathrm{d}p''\, \varphi^s(rp\,; r''p''\,; z)C^s(r''p''\,; r'p'\,; z) = \tilde{C}^s(rp\,; r'p'), \tag{9}$$

with $L_0(rp) = -(\mathrm{i}/m)p \cdot \nabla_r$ the free-particle streaming operator and φ^s a memory kernel. An expression for this kernel may be found from the equation of motion of the phase function $\delta f^s(rp\,; z)$ contained in C^s. In general the memory kernels for time correlation functions can be split into a static z-independent part that gives rise to a mean-field term in the kinetic equation,

and a dynamic part describing the effect of individual collisions. In the present case the static part of the kernel vanishes; the dynamic part can be brought into the form[8])

$$\varphi^s(\boldsymbol{r}_1\boldsymbol{p}_1;\boldsymbol{r}_1'\boldsymbol{p}_1';z)nf_0(\boldsymbol{p}_1') = -\int \mathrm{d}\boldsymbol{r}_2\,\mathrm{d}\boldsymbol{p}_2\,\mathrm{d}\boldsymbol{r}_2'\,\mathrm{d}\boldsymbol{p}_2'\,L_I(\boldsymbol{r}_1\boldsymbol{p}_1\boldsymbol{r}_2\boldsymbol{p}_2)$$
$$\times L_I(\boldsymbol{r}_1'\boldsymbol{p}_1'\boldsymbol{r}_2'\boldsymbol{p}_2')G^s_{2,2}(\boldsymbol{r}_1\boldsymbol{p}_1\boldsymbol{r}_2\boldsymbol{p}_2;\boldsymbol{r}_1'\boldsymbol{p}_1'\boldsymbol{r}_2'\boldsymbol{p}_2';z). \tag{10}$$

The operator L_I contains the potential v for the interaction between the particles in the fluid:

$$L_I(\boldsymbol{r}_1\boldsymbol{p}_1\boldsymbol{r}_2\boldsymbol{p}_2) = \mathrm{i}\,\nabla_{\boldsymbol{r}_1}v(\boldsymbol{r}_1-\boldsymbol{r}_2)\cdot(\nabla_{\boldsymbol{p}_1}-\nabla_{\boldsymbol{p}_2}). \tag{11}$$

Furthermore $G^s_{2,2}$ is a four-point function defined as

$$G^s_{2,2}(\boldsymbol{r}_1\boldsymbol{p}_1\boldsymbol{r}_2\boldsymbol{p}_2;\boldsymbol{r}_1'\boldsymbol{p}_1'\boldsymbol{r}_2'\boldsymbol{p}_2';z) = C^s_{2,2}(\boldsymbol{r}_1\boldsymbol{p}_1\boldsymbol{r}_2\boldsymbol{p}_2;\boldsymbol{r}_1'\boldsymbol{p}_1'\boldsymbol{r}_2'\boldsymbol{p}_2';z)$$
$$-\int \mathrm{d}\boldsymbol{r}_3\,\mathrm{d}\boldsymbol{p}_3\,\mathrm{d}\boldsymbol{r}_3'\,\mathrm{d}\boldsymbol{p}_3'\,C^s_{2,1}(\boldsymbol{r}_1\boldsymbol{p}_1\boldsymbol{r}_2\boldsymbol{p}_2;\boldsymbol{r}_3'\boldsymbol{p}_3';z)[C^s(\boldsymbol{r}_3'\boldsymbol{p}_3';\boldsymbol{r}_3\boldsymbol{p}_3;z)]^{-1}$$
$$\times C^s_{1,2}(\boldsymbol{r}_3\boldsymbol{p}_3;\boldsymbol{r}_1'\boldsymbol{p}_1'\boldsymbol{r}_2'\boldsymbol{p}_2';z), \tag{12}$$

with C^{s-1} the inverse of C^s. In the following we shall also need the four-point function $\tilde{G}^s_{2,2}$ that is found by replacing the functions C^s in (12) by their static counterparts $\tilde{C}^s$. Its explicit form is

$$\tilde{G}^s_{2,2}(\boldsymbol{r}_1\boldsymbol{p}_1\boldsymbol{r}_2\boldsymbol{p}_2;\boldsymbol{r}_1'\boldsymbol{p}_1'\boldsymbol{r}_2'\boldsymbol{p}_2') = \delta(\boldsymbol{r}_1-\boldsymbol{r}_1')\delta(\boldsymbol{p}_1-\boldsymbol{p}_1')n^2f_0(p_1)f_0(p_2)$$
$$\times\{\delta(\boldsymbol{r}_2-\boldsymbol{r}_2')\delta(\boldsymbol{p}_2-\boldsymbol{p}_2')g(\boldsymbol{r}_1-\boldsymbol{r}_2)$$
$$+nf_0(p_2')[g_3(\boldsymbol{r}_1-\boldsymbol{r}_2,\boldsymbol{r}_1-\boldsymbol{r}_2')-g(\boldsymbol{r}_1-\boldsymbol{r}_2)g(\boldsymbol{r}_1-\boldsymbol{r}_2')]\}, \tag{13}$$

where g_3 is the triplet correlation function.

A first approximation for the correlation function C^s is obtained from the kinetic equation (9) by retaining only the static part of the memory kernel. Since the latter is zero one recovers in this way the free-particle form of C^s. A higher approximation can be found[9–11]) by substituting in the dynamic part (10) of φ^s the mean-field expression for the four-point function $G^s_{2,2}$. This expression follows by solving formally the static-kernel approximation of the kinetic equation for $G^s_{2,2}$. In this way one finds from (10)

$$\varphi^s(\boldsymbol{r}_1\boldsymbol{p}_1;\boldsymbol{r}_1'\boldsymbol{p}_1';z)nf_0(\boldsymbol{p}_1')$$
$$= -\int \mathrm{d}\boldsymbol{r}_2\,\mathrm{d}\boldsymbol{p}_2\,\mathrm{d}\boldsymbol{r}_3\,\mathrm{d}\boldsymbol{p}_3\,\mathrm{d}\boldsymbol{r}_2'\,\mathrm{d}\boldsymbol{p}_2'\,\mathrm{d}\boldsymbol{r}_3'\,\mathrm{d}\boldsymbol{p}_3'\,V^s_I(\boldsymbol{r}_1\boldsymbol{p}_1;\boldsymbol{r}_2\boldsymbol{p}_2\boldsymbol{r}_3\boldsymbol{p}_3)$$
$$\times V^s_I(\boldsymbol{r}_1'\boldsymbol{p}_1';\boldsymbol{r}_2'\boldsymbol{p}_2'\boldsymbol{r}_3'\boldsymbol{p}_3')\tilde{G}^s_{2,2}(\boldsymbol{r}_2\boldsymbol{p}_2\boldsymbol{r}_3\boldsymbol{p}_3;\boldsymbol{r}_2'\boldsymbol{p}_2'\boldsymbol{r}_3'\boldsymbol{p}_3';z). \tag{14}$$

The vertex functions V^s_I have the form

$$V^s_I(\boldsymbol{r}_1\boldsymbol{p}_1;\boldsymbol{r}_2\boldsymbol{p}_2\boldsymbol{r}_3\boldsymbol{p}_3) = -n^2f_0(p_2)f_0(p_3)g(\boldsymbol{r}_2-\boldsymbol{r}_3)$$
$$\times\tilde{L}_I(\boldsymbol{r}_2\boldsymbol{p}_2\boldsymbol{r}_3\boldsymbol{p}_3)\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)\delta(\boldsymbol{p}_1-\boldsymbol{p}_2); \tag{15}$$

they contain the "renormalized" interaction operator $\tilde{L}_I$ defined as

$$\tilde{L}_I(r_1p_1r_2p_2) = -i\beta^{-1}[\nabla_{r_1} \ln g(r_1 - r_2)] \cdot (\nabla_{p_1} - \nabla_{p_2}). \tag{16}$$

The reduced four-point function $\bar{G}^s_{2,2}$ in (14) is determined implicitly by giving its inverse:

$$\begin{aligned}[\bar{G}^s_{2,2}(r_1p_1r_2p_2; r_1'p_1'r_2'p_2'; z)]^{-1} &= z\bar{G}^s_{2,2}(r_1p_1r_2p_2; r_1'p_1'r_2'p_2') \\ &- n^2 f_0(p_1)f_0(p_2)g(r_1 - r_2)[L_0(r_1p_1) + L_0(r_2p_2) + \tilde{L}_I(r_1p_1r_2p_2)] \\ &\times \delta(r_1 - r_1')\delta(p_1 - p_1')\delta(r_2 - r_2')\delta(p_2 - p_2') \\ &+ in^3\beta^{-1}f_0(p_1)f_0(p_2)f_0(p_2')[g_3(r_1 - r_2, r_1 - r_2') - g(r_1 - r_2)g(r_1 - r_2')] \\ &\times (\overleftarrow{\nabla}_{r_1} \cdot \nabla_{p_1} - \overleftarrow{\nabla}_{p_1} \cdot \nabla_{r_1})\delta(r_1 - r_1')\delta(p_1 - p_1');\end{aligned} \tag{17}$$

here the gradient operators $\overleftarrow{\nabla}$ are meant to act to the left only.

The kinetic equation that arises by substituting into (9) the second-order mean-field approximation (14)–(17) of the memory kernel is a suitable starting point for the discussion of a one-component plasma. Both the effects of close binary collisions between individual particles and of collective interactions that play an essential role in a plasma are contained in the memory kernel, as will be shown in the next section.

3. Generalized Boltzmann, Balescu–Guernsey–Lenard and Landau memory kernels for a plasma

The time correlation function for a dilute gas of neutral particles can be found by solving the Boltzmann equation in its linearized form. For a plasma the Boltzmann equation cannot be employed straightforwardly, since the ensuing collision integrals diverge owing to the long-range character of the Coulomb potential. A method to overcome this difficulty is to make use of the phenomenon of Debye shielding and to replace the bare Coulomb potential in the collision integrals by a Debye potential[12,13]). The resulting kinetic equation takes due account of the close binary collisions in the plasma but treats the collective effects only in an approximate way.

A Boltzmann-type memory kernel with an effective shielded potential can be found easily from the second-order mean-field memory kernel. In fact, if the inverse four-point function $\bar{G}^{s-1}_{2,2}$ given by (17) with (13) is approximated by retaining only the binary-collision terms one obtains

$$\begin{aligned}[\bar{G}^s_{2,2}(r_1p_1r_2p_2; r_1'p_1'r_2'p_2'; z)]^{-1} &= n^2 f_0(p_1)f_0(p_2)g(r_1 - r_2) \\ &\times [z - L_0(r_1p_1) - L_0(r_2p_2) - \tilde{L}_I(r_1p_1r_2p_2)] \\ &\delta(r_1 - r_1')\delta(p_1 - p_1')\delta(r_2 - r_2')\delta(p_2 - p_2').\end{aligned} \tag{18}$$

Upon insertion into (14) the memory function gets the form of a generalized Boltzmann kernel, *viz.*

$$\varphi_B^s(r_1p_1r_1'p_1';z)nf_0(p_1')$$
$$= -n^2\int \mathrm{d}r_2\,\mathrm{d}p_2\,\mathrm{d}r_2'\,\mathrm{d}p_2'\,\tilde{L}_I(r_1p_1r_2p_2)\tilde{L}_I(r_1'p_1'r_2'p_2')f_0(p_1)f_0(p_2)g(r_1-r_2)$$
$$[z-L_0(r_1p_1)-L_0(r_2p_2)-\tilde{L}_I(r_1p_1r_2p_2)]^{-1}\delta(r_1-r_1')\delta(p_1-p_1')\delta(r_2-r_2')\delta(p_2-p_2'), \tag{19}$$

in which $-\beta^{-1}\ln g$ is the effective pair potential. To evaluate the self-diffusion coefficient the time correlation function and hence the memory kernel is needed only for homogeneous systems, or in Fourier representation for $\boldsymbol{k}=0$; moreover the Markovian limit $z\to \mathrm{i}0$ has to be taken. In that case the kernel (19) can be shown[8,14]) to reduce to the Boltzmann form,

$$\varphi_B^s(\boldsymbol{k}=0,p_1p_1';z=\mathrm{i}0)nf_0(p_1') = -\mathrm{i}n^2\int \mathrm{d}\Omega\,\mathrm{d}p_2\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}$$
$$\times\frac{|p_1-p_2|}{m}f_0(p_1)f_0(p_2)[\delta(p_1-p_1')-\delta(p_1^{\dagger}-p_1')], \tag{20}$$

where $\mathrm{d}\sigma/\mathrm{d}\Omega$ is the differential cross section for a collision $p_1+p_2\to p_1^{\dagger}+p_2^{\dagger}$ of two particles that intereact according to the effective pair potential $-\beta^{-1}\ln g$. For dilute plasmas (with small plasma parameter) this effective potential indeed reduces to a Debye potential, since the pair correlation function is then given by its (nonlinear) Debye–Hückel form,

$$g(r)=\exp\left[-\frac{e^2}{4\pi r}\exp(-k_Dr)\right], \tag{21}$$

with $k_D^2=ne^2/kT$.

An alternative equation for a low-density plasma may be found from the BBGKY hierarchy by neglecting higher-order correlation functions[1]). The resulting Balescu–Guernsey–Lenard equation takes full account of the collective interactions in the plasma, but does not treat correctly the effects of individual collisions. In accordance with the latter fact the collision term contains an integral that diverges for small values of the interparticle separations.

A generalization of the Balescu–Guernsey–Lenard memory kernel can be obtained in the present formalism by disregarding in the four-point function $\bar{G}_{2,2}^{s-1}$ the correlations between the tagged particle and the field particles. Since the static four-point function $\tilde{G}^s$ given by (13) then becomes

$$\tilde{G}_{2,2}^s(r_1p_1r_2p_2;r_1'p_1'r_2'p_2') = \delta(r_1-r_1')\delta(p_1-p_1')n^2f_0(p_1)f_0(p_2)$$
$$\times\{\delta(r_2-r_2')\delta(p_2-p_2')+nf_0(p_2')[g(r_2-r_2')-1]\}, \tag{22}$$

one finds for $\bar{G}^{s-1}_{2,2}$ in this approximation

$$[\bar{G}^{s}_{2,2}(r_1p_1r_2p_2; r_1'p_1'r_2'p_2'; z)]^{-1} = n^2 f_0(p_1)f_0(p_2)$$
$$\times \{[z - L_0(r_1p_1) - L_0(r_2p_2)]\delta(r_2 - r_2')\delta(p_2 - p_2')$$
$$+ n[g(r_2 - r_2') - 1]f_0(p_2')[z - L_0(r_1p_1)]\}\delta(r_1 - r_1')\delta(p_1 - p_1'). \tag{23}$$

To evaluate the inverse of this function it is convenient to take a spatial Fourier transform according to the formula

$$[\bar{G}^{s}_{2,2}(k_1k_2q; p_1p_2p_1'p_2'; z)]^{-1} = V^{-1}\int dr_1\, dr_2\, dr_1'\, dr_2'$$
$$\exp[-ik_1 \cdot (r_1 - r_1') - ik_2 \cdot (r_2 - r_2') - iq \cdot (r_1 - r_2)]$$
$$\times [G^{s}_{2,2}(r_1p_1r_2p_2; r_1'p_1'r_2'p_2'; z)]^{-1}; \tag{24}$$

inverting the ensuing expression for $\bar{G}^{s-1}_{2,2}$ one finds then

$$\bar{G}^{s}_{2,2}(k_1k_2q; p_1p_2\ p_1'p_2'; z) = \frac{(2\pi)^3\delta(q)\delta(p_1 - p_1')}{nf_0(p_1)(z - k_1 \cdot p_1/m - k_2 \cdot p_2/m)}$$
$$\times \left[\frac{\delta(p_2 - p_2')}{nf_0(p_2)} - \frac{(z - k_1 \cdot p_1/m)c(k_2)}{\epsilon(k_2, z - k_1 \cdot p_1/m)(z - k_1 \cdot p_1/m - k_2 \cdot p_2'/m)}\right]. \tag{25}$$

Here $c(k)$ is the direct correlation function which is connected to the pair correlation function $h(k)$ through the Ornstein–Zernike relation $c(k) = h(k)/[1 + nh(k)]$. Furthermore the dielectric function $\epsilon(k, z)$ is defined as

$$\epsilon(k, z) = 1 + nc(k)[zF(k, z) - 1], \tag{26}$$

with the abbreviation

$$F(k, z) = \int dp\, f_0(p)/(z - k \cdot p/m). \tag{27}$$

Substitution of (25) into the Fourier transform of (14) leads to the following expression for the memory kernel:

$$\varphi^{s}_{BGL}(kpp'; z)nf_0(p') = \frac{n^2}{\beta^2}\int \frac{dq}{(2\pi)^3} h(q)c(q)q \cdot \nabla_p q \cdot \nabla_{p'}$$
$$\times \left\{\delta(p - p')f_0(p)\,\frac{F[q, z - (k - q) \cdot p/m]}{\epsilon[q, z - (k - q) \cdot p/m]}\right\}. \tag{28}$$

For $k = 0$, $z \to i0$ this expression becomes

$$\varphi^{s}_{BGL}(0, pp'; i0)nf_0(p') = -\frac{\pi i\, n^2}{\beta^2}\int \frac{dq}{(2\pi)^3}[c(q)]^2 q \cdot \nabla_p q \cdot \nabla_{p'}$$
$$\{\delta(p - p')f_0(p)|\epsilon(q, q \cdot p/m + i0)|^{-2}\int dp''\, f_0(p'')\delta[q \cdot (p - p'')/m]\}. \tag{29}$$

The memory kernels (28) and (29) have been obtained before by Gould and Mazenko[6]) in a somewhat different way. These authors introduce a 'disconnected approximation' (which amounts to the neglect of correlations between the tagged particle and the field particles) in an early stage of their treatment. Subsequently they use the free-particle approximation for C^s and an 'effective-interaction' approximation for the correlation function C of the field particles. In the present derivation we preferred as a starting point the memory kernel (14) in the second-order mean-field approximation in which both the effects of close binary collisions and of collective interactions are still taken into account.

For low-density plasmas the memory kernel (29) with (26) reduces to that of the (linearized) Balescu–Guernsey–Lenard equation, since the direct correlation function $c(q)$ can then be approximated by its Debye–Hückel form $-\beta e^2/q^2$. It should be remarked however that the memory kernel (29) is convergent for large values of q.

A generalization of the Landau memory kernel can likewise be derived easily in the present formalism[15]). It is found by considering the free-particle approximation of the inverse four-point function given in (17):

$$[\bar{G}^s_{2,2}(\boldsymbol{r}_1\boldsymbol{p}_1\boldsymbol{r}_2\boldsymbol{p}_2;\boldsymbol{r}_1'\boldsymbol{p}_1'\boldsymbol{r}_2'\boldsymbol{p}_2';z)]^{-1} = n^2 f_0(p_1)f_0(p_2) \times [z - L_0(\boldsymbol{r}_1\boldsymbol{p}_1) - L_0(\boldsymbol{r}_2\boldsymbol{p}_2)]\delta(\boldsymbol{r}_1 - \boldsymbol{r}_1')\delta(\boldsymbol{p}_1 - \boldsymbol{p}_1')\delta(\boldsymbol{r}_2 - \boldsymbol{r}_2')\delta(\boldsymbol{p}_2 - \boldsymbol{p}_2'). \tag{30}$$

Alternatively, this formula may be obtained either from the inverse four-point function (18) of the generalized Boltzmann kernel, namely by neglecting the correlations between the tagged and the field particles, or from the expression (23) of the generalized Balescu–Guernsey–Lenard kernel, by taking the binary collision terms. The resulting memory kernel will therefore be an approximation to both of these kernels, as is the case for the corresponding kinetic equations of a low-density plasma.

The Fourier transformed inverse of (30) gets the form

$$\bar{G}^s_{2,2}(\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{q};\boldsymbol{p}_1\boldsymbol{p}_2\boldsymbol{p}_1'\boldsymbol{p}_2';z) = \frac{(2\pi)^3\delta(\boldsymbol{q})\delta(\boldsymbol{p}_1 - \boldsymbol{p}_1')\delta(\boldsymbol{p}_2 - \boldsymbol{p}_2')}{n^2 f_0(p_1)f_0(p_2)(z - \boldsymbol{k}_1\cdot\boldsymbol{p}_1/m - \boldsymbol{k}_2\cdot\boldsymbol{p}_2/m)}, \tag{31}$$

which yields upon insertion into (14) the memory kernel

$$\varphi^s_{\mathrm{L}}(\boldsymbol{k}\boldsymbol{p}\boldsymbol{p}';z)nf_0(p') = \frac{n^2}{\beta^2}\int \frac{\mathrm{d}\boldsymbol{q}}{(2\pi)^3}[h(q)]^2\boldsymbol{q}\cdot\nabla_{\boldsymbol{p}}\boldsymbol{q}\cdot\nabla_{\boldsymbol{p}'} \times \{\delta(\boldsymbol{p} - \boldsymbol{p}')f_0(p)F[\boldsymbol{q}, z - (\boldsymbol{k} - \boldsymbol{q})\cdot\boldsymbol{p}/m]\}, \tag{32}$$

with F given in (27). For $\boldsymbol{k} = 0$, $z \to \mathrm{i}0$, one arrives at the Landau-type kernel

$$\varphi^s_{\mathrm{L}}(0, \boldsymbol{p}\boldsymbol{p}';\mathrm{i}0)nf_0(p') = -\frac{\pi i n^2}{\beta^2}\int \frac{\mathrm{d}\boldsymbol{q}}{(2\pi)^3}[h(q)]^2\boldsymbol{q}\cdot\nabla_{\boldsymbol{p}}\boldsymbol{q}\cdot\nabla_{\boldsymbol{p}'} \times \{\delta(\boldsymbol{p} - \boldsymbol{p}')f_0(p)\int \mathrm{d}\boldsymbol{p}''\, f_0(p'')\delta[\boldsymbol{q}\cdot(\boldsymbol{p} - \boldsymbol{p}'')/m]\}. \tag{33}$$

An alternative form results by performing the angular integrations:

$$\varphi^s_L(0, \boldsymbol{pp}'; i0) n f_0(p') = -\frac{in^2}{8\pi\beta^2} \int_0^\infty d\boldsymbol{q}\, q^3 [h(q)]^2$$

$$\nabla_p \nabla_{p'} : \left\{ \delta(\boldsymbol{p} - \boldsymbol{p}') f_0(p) \int d\boldsymbol{p}''\, f_0(p'') \frac{m}{|\boldsymbol{p} - \boldsymbol{p}''|} \left[\mathsf{U} - \frac{(\boldsymbol{p} - \boldsymbol{p}'')(\boldsymbol{p} - \boldsymbol{p}'')}{(\boldsymbol{p} - \boldsymbol{p}'')^2} \right] \right\}. \quad (34)$$

A comparison of (33) with (29) shows that dynamic screening effects caused by the dielectric function ϵ are missing here, while the correlation function $h(q)$ takes the place of the direct correlation function $c(q)$. In the Debye–Hückel limit the kernel (33) reduces to the ordinary Landau kernel, with a screened potential $-\beta^{-1}h(q) = e^2/(q^2 + k_D^2)$. Of course, (33) or (34) may also be obtained from the Boltzmann kernel (20) by evaluating the contribution of small-angle scattering in the tail $-\beta^{-1}h(r)$ of the effective potential $-\beta^{-1} \ln g(r)$.

4. Symmetries, conservation laws and sum rules for the memory kernel

The invariance of the N-particle Hamiltonian with respect to translation, rotation and reflection in space and time implies symmetries of the memory kernel for the time correlation function[15]). In fact, from (10)–(12) with (3) one may prove the symmetries

$$\varphi^s(\boldsymbol{kpp}'; z) = \varphi^s(-\boldsymbol{k}, -\boldsymbol{p}, -\boldsymbol{p}'; z), \quad (35)$$

$$\varphi^s(\boldsymbol{kpp}'; z) f_0(p') = \varphi^s(-\boldsymbol{k}, -\boldsymbol{p}', -\boldsymbol{p}; z) f_0(p), \quad (36)$$

as a result of parity invariance and of the invariance under the combined effect of time translation and time reversal. The reality of the correlation functions gives moreover

$$\varphi^s(\boldsymbol{kpp}'; z) = -[\varphi^s(-\boldsymbol{k}, \boldsymbol{pp}'; -z^*)]^*. \quad (37)$$

All these relations are indeed satisfied both by the second-order mean-field kernel (14) and by its approximations (20), (29) and (33).

The motion of the tagged particle does not conserve its momentum and energy; only the tagged-particle number is trivially conserved. The latter property leads with (9) to the conservation law[15])

$$\int d\boldsymbol{p}\, \varphi^s(\boldsymbol{kpp}'; z) = 0, \quad (38)$$

which is satisfied by the second-order mean-field kernel (14) and also by (20), (29) and (33).

Sum rules for the memory kernel follow by considering the short-time behaviour of the time correlation function. The first few time derivatives of C^s can on the one hand be calculated directly from (1) and follow on the other hand from the kinetic equation (9). A comparison leads to sum rules for the memory kernel the first of which has the form[15,16])

$$\lim_{z\to\infty} z\varphi^s(\boldsymbol{kpp}';z)nf_0(p') = -\frac{n^2e^2}{3\beta}\int\frac{\mathrm{d}\boldsymbol{q}}{(2\pi)^3}h(q)\nabla_{\boldsymbol{p}}\cdot\nabla_{\boldsymbol{p}'}f_0(p)\delta(\boldsymbol{p}-\boldsymbol{p}'). \tag{39}$$

If this sum rule is fulfilled by an approximate kernel the ensuing time correlation function C^s has a correct first and second time derivative at $t = 0$; the van Hove self-correlation function (obtained from C^s by integrating over the momenta) then has correct derivatives up to fourth order.

The second-order mean-field approximation (14) of the memory kernel indeed satisfies the sum rule (39), as follows from the asymptotic relation $\lim_{z\to\infty} z\bar{G}^{s-1}_{2,2} = \tilde{G}^{s-1}_{2,2}$ and the explicit form (13) for $\tilde{G}^s_{2,2}$. In contrast, neither of the approximate forms that have been discussed in the previous section are compatible with (39). From the generalized Boltzmann kernel (19) one obtains

$$\lim_{z\to\infty} z\varphi^s_{\mathrm{B}}(\boldsymbol{kpp}';z)nf_0(p') = \frac{n^2}{3\beta^2}\int\frac{\mathrm{d}\boldsymbol{q}}{(2\pi)^3}q^2h(q) \times[\ln g(r)](q)\nabla_{\boldsymbol{p}}\cdot\nabla_{\boldsymbol{p}'}f_0(p)\delta(\boldsymbol{p}-\boldsymbol{p}'), \tag{40}$$

where $[\ln g(r)](q)$ denotes the Fourier transform of $\ln g(r)$. The generalized Balescu–Guernsey–Lenard kernel (28) gives, since $\lim_{z\to\infty} zF(k,z) = 1$ and $\lim_{z\to\infty}\epsilon(k,z) = 1$,

$$\lim_{z\to\infty} z\varphi^s_{\mathrm{BGL}}(\boldsymbol{kpp}';z)nf_0(p') = \frac{n^2}{3\beta^2}\int\frac{\mathrm{d}\boldsymbol{q}}{(2\pi)^3}q^2h(q)c(q)\nabla_{\boldsymbol{p}}\cdot\nabla_{\boldsymbol{p}'}f_0(p)\delta(\boldsymbol{p}-\boldsymbol{p}'). \tag{41}$$

Finally, the generalized Landau kernel (32) leads to the sum rule

$$\lim_{z\to\infty} z\varphi^s_{\mathrm{L}}(\boldsymbol{kpp}';z)nf_0(p') = \frac{n^2}{3\beta^2}\int\frac{\mathrm{d}\boldsymbol{q}}{(2\pi)^3}q^2[h(q)]^2\nabla_{\boldsymbol{p}}\cdot\nabla_{\boldsymbol{p}'}f_0(p)\delta(\boldsymbol{p}-\boldsymbol{p}'). \tag{42}$$

All three approximations to the second-order mean-field kernel thus lead to time correlation functions with an incorrect behaviour for small t.

5. Introduction of a composite memory kernel

In the last two sections several approximate kernels for the time correlation functions of a one-component plasma have been discussed. All of these are

free of the divergencies that are frequently encountered in the kinetic theory for a low-density plasma. In spite of the absence of such divergencies neither of the approximate kernels give a correct treatment of both the close binary collisions and the collective interactions in the plasma. In the generalized Boltzmann kernel the collective effects are only partially taken into account by the use of an effective potential, while in the generalized Balescu–Guernsey–Lenard kernel typical binary-collision terms are missing altogether; the generalized Landau kernel, as a hybrid approximation, has the defects of both of the other kernels. A further symptom of the approximate nature of the kernels is the deviating form of the lowest-order sum rule.

In the kinetic theory of low-density plasmas a better treatment of the various types of interactions between the particles can be achieved by combining the various collision integrals in a suitable way, as has been shown by Baldwin[2]) and others[3]) for the one-particle kinetic equations, and by Bartis and Oppenheim[4]) for the equation satisfied by the time correlation function. For a moderately dense plasma a similar method may be followed to arrive at an improved approximation for the memory kernel φ^s as given by (14)–(17).

Let us split off from the complete kernel φ^s the part that describes the close binary collisions, *i.e.* the generalized Boltzmann kernel:

$$\varphi^s = \varphi^s_B + (\varphi^s - \varphi^s_B). \tag{43}$$

The second term at the right-hand side takes account of the effects of collective interactions in the plasma that are not contained in φ^s_B. As an approximation one may neglect in that term the correlations between the tagged particle and the field particles; these correlations are retained in the first term. When the correlations are suppressed φ^s reduces to φ^s_{BGL} and φ^s_B to φ^s_L, so that one ends up with the composite memory kernel

$$\varphi^s_C = \varphi^s_B + \varphi^s_{BGL} - \varphi^s_L. \tag{44}$$

For a low-density plasma in which the pair correlation function may be approximated by its Debye–Hückel form the kernel (44) reduces to that derived by Bartis and Oppenheim[4]).

The short-time behaviour of the composite kernel follows directly from the sum rules (40), (41) and (42) for its constituents:

$$\lim_{z\to\infty} z\varphi^s_C(\boldsymbol{kpp}';z)nf_0(p') = \frac{n^2}{3\beta^2}\int \frac{d\boldsymbol{q}}{(2\pi)^3}\, q^2 h(q)\{[\ln g(r)](q) + c(q) - h(q)\}\nabla_p \cdot \nabla_{p'} f_0(p)\delta(\boldsymbol{p}-\boldsymbol{p}'). \tag{45}$$

Comparison with the exact sum rule (39) shows that the composite kernel has the correct short-time behaviour if the pair correlation functions satisfy the

identity in coordinate space

$$\ln g(r) + c(r) - h(r) = -\beta e^2/4\pi r. \tag{46}$$

This is the basic equation of the hypernetted-chain (HNC) approximation[17]) for the static pair correlation function of a plasma. Empirically it is a well-established fact that the HNC-approximation leads to static correlation functions that compare favourably with the results of Monte Carlo calculations[5]). By virtue of this property the composite kernel (44) satisfies the first sum rule to a fair approximation so that the correct short-time behaviour of the ensuing time correlation functions is guaranteed.

In recent papers[7]) an approximate memory kernel for the full time correlation functions C has been proposed which likewise has the virtue of satisfying the first-order sum rule. The analogous memory kernel for the tagged-particle problem may be obtained along lines similar to that of sections 2 and 3. First the memory kernel φ^s is written in a form similar to but slightly different from (14); one of the vertex functions V_I^s is replaced by the interaction operator L_I and, correspondingly, the four-point function $\bar{G}_{2,2}^s$ is transformed into a function $\bar{\bar{G}}_{2,2}^s$, which is in fact the product of $\bar{G}_{2,2}^s$ and $\tilde{G}_{2,2}^s$. When subsequently the correlations between the tagged particle and the field particles are disregarded in $\bar{\bar{G}}_{2,2}^s$ one ends up with a memory kernel φ_{WB}^s that resembles (28) or (29), apart from an extra factor $-\beta e^2/[q^2 c(q)]$ inside the integral. Instead of (29) one finds

$$\varphi_{\mathrm{WB}}^s(0, pp'; \mathrm{i}0) n f_0(p') = \frac{\pi i e^2 n^2}{\beta} \int \frac{\mathrm{d}q}{(2\pi)^3} \frac{c(q)}{q^2} q \cdot \nabla_p q \cdot \nabla_{p'}$$
$$\left\{ \delta(p - p') f_0(p) |\epsilon(q, q \cdot p/m + \mathrm{i}0)|^{-2} \int \mathrm{d}p'' \, f_0(p'') \delta[q \cdot (p - p'')/m] \right\}. \tag{47}$$

The sum rule for this modified kernel follows by inserting the same extra factor as above into the BGL sum rule (41), so that the exact sum rule (39) is indeed recovered. The modified kernel φ_{WB}^s may thus be considered as an improved version of the generalized Balescu–Guernsey–Lenard kernel. It should be remarked however, that the neglect of correlations between the tagged particle and the field particles implies that close binary collisions in the plasma are again not treated adequately. The consequences of this fact will be discussed in the next section, where the relative merits of the various approximate kernels will be assessed through an evaluation of the self-diffusion coefficient.

6. Evaluation of the self-diffusion coefficient

The self-diffusion coefficient D follows from the time correlation function C^s by using the Green–Kubo relation (8). Introducing in that relation dimen-

sionless velocities $\boldsymbol{\xi} = \boldsymbol{p}/(mv_0)$, with $v_0 = (m\beta)^{-1/2}$ and writing the Fourier-transformed correlation function as $C^s(\boldsymbol{k}\boldsymbol{\xi}\boldsymbol{\xi}'; z) = (m/\beta)^3\, C^s(\boldsymbol{k}\boldsymbol{p}\boldsymbol{p}'; z)$ one gets

$$D = \lim_{z \to i0} in^{-1} v_0^2 \int d\boldsymbol{\xi}\, d\boldsymbol{\xi}'\, \xi_z \xi_z' C^s(\boldsymbol{k} = 0, \boldsymbol{\xi}\boldsymbol{\xi}'; z). \tag{48}$$

The kinetic equation (9) reads in the new variables

$$(z - v_0 \boldsymbol{k} \cdot \boldsymbol{\xi}) C^s(\boldsymbol{k}\boldsymbol{\xi}\boldsymbol{\xi}'; z) - \int d\boldsymbol{\xi}''\, \varphi^s(\boldsymbol{k}\boldsymbol{\xi}\boldsymbol{\xi}''; z) C^s(\boldsymbol{k}\boldsymbol{\xi}''\boldsymbol{\xi}'; z)$$
$$= nF(\xi)\delta(\boldsymbol{\xi} - \boldsymbol{\xi}'), \tag{49}$$

with $\varphi^s(\boldsymbol{k}\boldsymbol{\xi}\boldsymbol{\xi}'; z) = (mv_0)^3\, \varphi^s(\boldsymbol{k}\boldsymbol{p}\boldsymbol{p}'; z)$ and $F(\xi) = (2\pi)^{-3/2} \exp(-\frac{1}{2}\xi^2)$. Upon introducing a complete set of functions $\{f_\alpha(\boldsymbol{\xi})\}$ in velocity space, such that

$$\int d\boldsymbol{\xi} f_\alpha(\boldsymbol{\xi}) f_\beta^*(\boldsymbol{\xi}) F(\xi) = \delta_{\alpha\beta}, \tag{50}$$

$$\sum_\alpha f_\alpha(\boldsymbol{\xi}) f_\alpha^*(\boldsymbol{\xi}') F(\xi) = \delta(\boldsymbol{\xi} - \boldsymbol{\xi}'), \tag{51}$$

the kinetic equation for $\boldsymbol{k} = 0$, $z = i0$ may be written as a set of algebraic equations

$$\sum_\gamma \varphi^s_{\alpha\gamma} C^s_{\gamma\beta} = -n\delta_{\alpha\beta}, \tag{52}$$

with the matrix elements

$$\varphi^s_{\alpha\beta} = \int d\boldsymbol{\xi}\, d\boldsymbol{\xi}'\, f_\alpha^*(\boldsymbol{\xi}) \varphi^s(0, \boldsymbol{\xi}\boldsymbol{\xi}'; i0) f_\beta(\boldsymbol{\xi}') F(\xi'), \tag{53}$$

$$C^s_{\alpha\beta} = \int d\boldsymbol{\xi}\, d\boldsymbol{\xi}'\, f_\alpha^*(\boldsymbol{\xi}) C^s(0, \boldsymbol{\xi}\boldsymbol{\xi}'; i0) f_\beta(\boldsymbol{\xi}'). \tag{54}$$

A convenient set of orthonormal functions in velocity space is

$$f_\alpha(\boldsymbol{\xi}) = c_{klm} \xi^l S^{(k)}_{l+1/2}(\tfrac{1}{2}\xi^2) Y_l^m(\hat{\boldsymbol{\xi}}), \tag{55}$$

with k, l and m non-negative integers, $S^{(k)}_{l+1/2}$ Sonine polynomials, Y_l^m spherical harmonics depending on $\hat{\boldsymbol{\xi}} = \boldsymbol{\xi}/|\boldsymbol{\xi}|$ and $C_{klm} = 2^{-(l-1)/2} \pi^{3/4} [k!/(k + l + \frac{1}{2})!]^{1/2}$ normalization constants. Rotation invariance implies that $\varphi^s_{\alpha\beta}$ is diagonal in the indices l and m. Since the self-diffusion coefficient is according to (48) proportional to $C^s_{\alpha\beta}$ with $\alpha = \beta = (k, l, m) = (0,1,0)$ the kinetic equation (52) has to be solved for $l = 1$, $m = 0$; omitting these indices one may write it as

$$\sum_{k''} \varphi^s_{kk''} C^s_{k''k'} = -n\delta_{kk'}. \tag{56}$$

An approximate solution of this infinite set of equations is obtained by the

well-known truncation method. The lowest 1-Sonine approximation gives the self-diffusion coefficient as

$$D^{(0)} = -\mathrm{i}v_0^2/\varphi^s_{00}, \tag{57}$$

while in the next approximation one gets

$$D^{(1)} = D^{(0)}/(1-\Delta), \tag{58}$$

with the correction term

$$\Delta = (\varphi^s_{01})^2/(\varphi^s_{00}\varphi^s_{11}). \tag{59}$$

The evaluation of the lowest-order matrix elements of φ^s proceeds by inserting the polynomials $f_{010} = \xi_z$ and $f_{110} = (1-\frac{1}{5}\xi^2)\xi_z$ into (53). The results have the form

$$\varphi^s_{kk'} = -[\mathrm{i}v_0^2/(\omega_p a^2)]\bar{\varphi}^s_{kk'}, \tag{60}$$

with $\omega_p = (ne^2/m)^{1/2}$ the plasma frequency, $a = [3/(4\pi n)]^{1/3}$ the average interparticle distance and $\bar{\varphi}^s_{kk'}$ a dimensionless matrix element.

For the Boltzmann kernel (20) one obtains by standard manipulations[18])

$$\bar{\varphi}^s_{B,00} = \frac{2}{\pi}\left(\frac{3\Gamma}{\pi}\right)^{1/2}\Omega^{(1,1)}, \tag{61}$$

$$\bar{\varphi}^s_{B,01} = \frac{1}{\pi}\left(\frac{3\Gamma}{\pi}\right)^{1/2}[\Omega^{(1,1)} - \tfrac{2}{5}\Omega^{(1,2)}], \tag{62}$$

$$\bar{\varphi}^s_{B,11} = \frac{1}{\pi}\left(\frac{3\Gamma}{\pi}\right)^{1/2}[\tfrac{11}{10}\Omega^{(1,1)} - \tfrac{2}{5}\Omega^{(1,2)} + \tfrac{2}{25}\Omega^{(1,3)} + \tfrac{4}{25}\Omega^{(2,2)}], \tag{63}$$

with Γ the plasma parameter $e^2\beta/(4\pi a)$. The collision integrals defined as

$$\Omega^{(l,s)} = a^{-2}\int \mathrm{d}x\, \mathrm{e}^{-x^2}x^{2s+3}\int \mathrm{d}\Omega(1-\cos^l\theta)\,\mathrm{d}\sigma(\theta,x)/\mathrm{d}\Omega \tag{64}$$

contain a scattering cross-section $\mathrm{d}\sigma/\mathrm{d}\Omega$ that measures the probability of a binary collision $\boldsymbol{p}_1 + \boldsymbol{p}_2 \to \boldsymbol{p}_1^* + \boldsymbol{p}_2^*$ (with solid angle Ω between $\boldsymbol{p}_1$ and $\boldsymbol{p}_1^*$ and with relative velocity $|\boldsymbol{p}_1 - \boldsymbol{p}_2|/m = 2v_0 x$) under the influence of the effective potential $-\beta^{-1}\ln g(r)$.

The matrix elements of the generalized Balescu–Guernsey–Lenard kernel follow by inserting (29) into (53). The square of the dielectric function (26) that occurs in (29) may be written as

$$|\epsilon(q, \boldsymbol{q}\cdot\boldsymbol{p}/m + \mathrm{i}0)|^2 = [S(k)]^{-2}|D(k,x)|^2; \tag{65}$$

here $S(k) = [1 - nc(k)]^{-1}$ is the structure factor depending on the dimension-

less Fourier variable $k = qa$, while $D(k, x)$ is defined as

$$D(k, x) = 1 + [S(k) - 1]\left[\sqrt{2}x\psi\left(\frac{x}{\sqrt{2}}\right) - i\sqrt{\frac{\pi}{2}}\, x\, e^{-x^2/2}\right], \tag{66}$$

with $\psi(x) = \int_0^x dt\ \exp(t^2 - x^2)$ Dawson's integral and $x = \hat{q} \cdot p/mv_0 = \hat{q} \cdot \xi$ the longitudinal velocity component. The dimensionless matrix elements that are obtained after integration over the transverse components of the velocities have the form

$$\bar{\varphi}^s_{\mathrm{BGL},ij} = \frac{2}{3\pi}\left(\frac{\Gamma}{3}\right)^{1/2} \int_0^\infty dk \int_0^\infty dx\, \frac{k^3[S(k) - 1]^2}{|D(k, x)|^2}\, e^{-x^2} P_{ij}(x), \tag{67}$$

with the polynomials

$$P_{00}(x) = 1, \tag{68}$$

$$P_{01}(x) = -\tfrac{3}{5}x^2 + \tfrac{3}{5}, \tag{69}$$

$$P_{11}(x) = \tfrac{9}{25}x^4 - \tfrac{2}{5}x^2 + \tfrac{13}{25}. \tag{70}$$

The matrix elements of the generalized Landau memory kernel may be obtained from (67) by replacing $|D(k, x)|^2$ by 1, as follows by comparing (29) with (33) and using (65) with $S(k) = h(k)/c(k)$. Upon performing the integrals over x one gets in this way

$$\bar{\varphi}^s_{\mathrm{L},ij} = \tfrac{1}{3}\left(\frac{\Gamma}{3\pi}\right)^{1/2} \int_0^\infty dk\, k^3[S(k) - 1]^2 c_{ij}, \tag{71}$$

with the coefficients $c_{00} = 1$, $c_{01} = 3/10$, $c_{11} = 59/100$.

The explicit evaluation of the matrix elements of the memory kernels requires a knowledge of the static properties of the plasma, as given by the pair correlation function and the structure function. For moderately dense plasmas, with plasma parameter satisfying $0.1 < \Gamma < 2$, a fair approximation to these functions is obtained by solving the hypernetted-chain equation. This equation is equivalent to the set of relations[19,20])

$$g(r) = \exp\left[d_s(r) - \frac{\Gamma}{r} + f(r)\right], \tag{72}$$

$$c_s(r) = g(r) - 1 - d_s(r), \tag{73}$$

$$d_s(k) = \frac{c_s(k) - f(k)}{1 - (3/4\pi)[c_s(k) - f(k)]} - c_s(k), \tag{74}$$

connecting the pair correlation functions $c(r)$, $g(r)$, the difference function

$d(r) = g(r) - 1 - c(r)$ and their Fourier transforms (all distances r are measured in units a, the Fourier variables k in units a^{-1}). To avoid numerical difficulties resulting from the long-range character of the functions both $c(r)$ and $d(r)$ have been split into a long-range and a short-range part by writing $c(r) = c_s(r) - f(r)$, $d(r) = d_s(r) + f(r)$. Good choices for the auxiliary function $f(r)$ are $f(r) = (\Gamma/r)\,[1 - \exp(-\alpha r)]$, with $\alpha \approx (3\Gamma)^{1/2}$ or $f(r) = (\Gamma/r)\,\mathrm{erf}(\alpha r)$, with $\alpha \approx 1.1$. Both of these functions have been used in the present work. The equations (72)–(74) can be solved efficiently by iteration, if use is made of fast Fourier transform techniques. Several thousands of points were used in these transforms, while the spacings Δr and Δk were chosen in the order of 0.02 and 0.1, respectively. A few iterations are sufficient to yield values for $g(r)$ with an error less than 10^{-6}, at least if a suitable convergence accelerating mechanism is employed[20]).

A modification of the HNC equations that leads to slightly improved values for the static properties of a one-component plasma has been proposed recently[21]). In this MHNC approximation the so-called 'bridge diagram' contributions that are omitted in the HNC equations are taken into account by employing the pair correlation functions for a hard-sphere system. In fact, the relation (72) is replaced by the equation

$$g(r) = \exp\left[d_s(r) - \frac{\Gamma}{r} + f(r) + b(r) \right], \tag{75}$$

with $b(r)$ following from the exact solution of the Percus–Yevick equation for hard spheres[22]):

$$b(r) = c_{HS}(r) + 1 + \ln[-c_{HS}(r)], \quad r < (8\eta)^{1/3}, \tag{76}$$

$$= -g_{HS}(r) + 1 + \ln[g_{HS}(r)], \quad r > (8\eta)^{1/3}. \tag{77}$$

The packing fraction η must be considered as an adjustable parameter chosen so as to yield an optimal fit to the Monte Carlo data[23,24]). For $\Gamma = 1$ and $\Gamma = 2$ the values $\eta = 0.035$ and $\eta = 0.075$, respectively, have been chosen, while for $\Gamma < 1$ the available Monte Carlo data are compatible with the pure HNC equation ($\eta = 0$).

The integrals $\Omega^{(l,s)}$ (64) that describe binary collisions in the effective potential $-\beta \ln g(r)$ have been evaluated by the usual methods[25]). The potential is determined from its values at a discrete set of points (obtained by solving the HNC or MHNC equations) with the help of Aitken's interpolation method. For small Γ ($\Gamma \leq 1$) the effective potential turns out to be a monotonically decreasing function of the separation r. When Γ increases the potential starts oscillating; for $\Gamma \leq 2$ the amplitude of these oscillations is small, however, so that the potential may be assumed to vanish for all $r > r_0$, with r_0 the first zero of the potential. For higher Γ this approximation can not be

justified. The evaluation of the collision integrals then becomes a complicated numerical task, especially when the number of oscillations in the potential gets large. We have limited ourselves therefore to the study of moderately dense plasmas with $\Gamma \leqslant 2$.

For small Γ the effective pair potential may be approximated by its Debye–Hückel form (21), which reads in the present units $-\beta^{-1} \ln g = (\Gamma/r) \exp[-(3\Gamma)^{1/2} r]$. The collision integrals for screened potentials of this type are available in the literature[26]); to facilitate a comparison they have been recalculated for a number of Γ values.

The matrix elements $\bar{\varphi}^{s}_{B,ij}$ of the Boltzmann-type kernel that follow through (61)–(63) from the collision integrals in the (modified) HNC and the Debye–Hückel approximation have been compiled in table I. It turns out that the difference between the HNC and MHNC values is always less than a few percent; the HNC and DH matrix elements differ only 1% for $\Gamma = 0.1$, but already 15% for $\Gamma = 0.5$. For $\Gamma = 0.1$ and 0.2 the table also gives the approximate values for $\bar{\varphi}^{s}_{B,ij}$ that follow[12,13]) from the leading terms of the Debye–Hückel collision integrals for small Γ; this ADH approximation to the matrix elements has the form

$$\bar{\varphi}^{s}_{B,ij} = \left(\frac{3}{\pi}\right)^{1/2} \Gamma^{5/2} [-c_{ij} \ln(\sqrt{3}\Gamma^{3/2}) - d_{ij}], \tag{78}$$

Table I

Matrix elements of the generalized Boltzmann kernel $\bar{\varphi}^{s}_{B}$ and the generalized Balescu–Guernsey–Lenard kernel $\bar{\varphi}^{s}_{BGL}$, as obtained from the static pair correlation function in the hypernetted-chain approximation (HNC), the modified hypernetted-chain approximation (MHNC), the Debye–Hückel theory (DH) or the approximate Debye–Hückel theory (ADH)

		$\bar{\varphi}^{s}_{B,00}$	$\bar{\varphi}^{s}_{B,01}$	$\bar{\varphi}^{s}_{B,11}$	$\bar{\varphi}^{s}_{BGL,00}$	$\bar{\varphi}^{s}_{BGL,01}$	$\bar{\varphi}^{s}_{BGL,11}$
$\Gamma = 0.1$	HNC	0.00815	0.00185	0.00482	0.00632	0.00152	0.00423
	DH	0.00804	0.00182	0.00476	0.00805	0.00201	0.00528
	ADH	0.00815	0.00183	0.00481	0.00805	0.00201	0.00528
$\Gamma = 0.2$	HNC	0.0304	0.00615	0.0180	0.0230	0.00497	0.0162
	DH	0.0291	0.00585	0.0173	0.0276	0.00603	0.0192
	ADH	0.0279	0.00487	0.0165	0.0273	0.00590	0.0191
$\Gamma = 0.5$	HNC	0.145	0.0227	0.0861	0.109	0.0179	0.0856
	DH	0.125	0.0193	0.0746	0.0691	0.00470	0.0648
$\Gamma = 1$	HNC	0.402	0.0465	0.240	0.311	0.0344	0.276
	MHNC	0.404	0.0464	0.242	0.312	0.0346	0.277
$\Gamma = 2$	HNC	0.982	0.0718	0.590	0.804	0.0395	0.822
	MHNC	1.00	0.0708	0.601	0.820	0.0408	0.836

with coefficients c_{ij} defined below (71), and with $d_{00} = 0.2681$, $d_{01} = 0.2804$ and $d_{11} = 0.1582$. As expected these approximate Debye–Hückel values are quite accurate for $\Gamma = 0.1$, but are less reliable already for $\Gamma = 0.2$.

The matrix elements of the generalized Balescu–Guernsey–Lenard kernel (67) may be evaluated by numerical integration once the values of the structure function are known, either from the modified HNC equation or in the Debye–Hückel approximation (see table I). When the latter values are employed, so that $S(k) = k^2/(k^2 + 3\Gamma)$, the double integral diverges for large k; as a cut-off one may take $k_0 = \Gamma^{-1}$, for $\Gamma < 1$. The integral over k can then be carried out analytically, since one has

$$\int_0^{\Gamma^{-1}} \mathrm{d}k \, \frac{k^3[S(k)-1]^2}{|D(k,x)|^2} = \tfrac{9}{4}\Gamma^2 \ln\left[\frac{(1/9)\Gamma^{-6} + (2/3)\Gamma^{-3}A + A^2 + B^2}{A^2 + B^2}\right]$$

$$- \tfrac{9}{2}\Gamma^2 \frac{A}{B}\left[\operatorname{arctg}\left(\frac{(1/3)\Gamma^{-3} + A}{B}\right) - \operatorname{arctg}\left(\frac{A}{B}\right)\right], \tag{79}$$

with the abbreviations

$$A(x) = 1 - \sqrt{2}x \, \mathrm{e}^{-x^2/2}\psi\left(\frac{x}{\sqrt{2}}\right), \tag{80}$$

$$B(x) = \left(\frac{\pi}{2}\right)^{1/2} x \, \mathrm{e}^{-x^2/2}. \tag{81}$$

For small Γ only the leading terms of the expansion in powers of Γ need be retained in (79). A numerical evaluation of the integral over x then gives

$$\bar{\varphi}^{s}_{\mathrm{BGL},ij} = \left(\frac{3}{\pi}\right)^{1/2} \Gamma^{5/2}\left[-c_{ij} \ln(\sqrt{3}\Gamma^{3/2}) - d'_{ij}\right]; \tag{82}$$

the coefficients c_{ij} have been defined below (71), while the numerical integrations yield $d'_{00} = 0.3008$, $d'_{01} = 0.2221$, and $d'_{11} = 0.00624$. It should be remarked here that the lowest-order matrix elements of the ordinary Balescu–Guernsey–Lenard kernel (which is equivalent to the generalized BGL kernel in the Debye–Hückel approximation) have been evaluated previously along similar lines[27]); the leading terms in the expansions are not treated consistently, however, in these papers, so that the results for $\bar{\varphi}^{s}_{ij}$ do not agree with those given in (82).

The generalized Landau kernel leads to a set of matrix elements (71) that are all proportional to a single integral over the structure function $S(k)$. The numerical evaluation of this integral is quite straightforward, if the HNC values for $S(k)$ are inserted (see table II). The use of the Debye–Hückel structure function gives rise to an integral that can be performed analytically;

Table II
Matrix elements of the generalized Landau kernel $\bar{\varphi}^s_L$ and the modified Balescu–Guernsey–Lenard kernel $\bar{\varphi}^s_{WB}$

		$\bar{\varphi}^s_{L,00}$	$\bar{\varphi}^s_{L,01}$	$\bar{\varphi}^s_{L,11}$	$\bar{\varphi}^s_{WB,00}$	$\bar{\varphi}^s_{WB,01}$	$\bar{\varphi}^s_{WB,11}$
$\Gamma = 0.1$	HNC	0.00577	0.00173	0.00340	0.00822	0.00208	0.00537
	DH	0.00744	0.00223	0.00439	0.00805	0.00201	0.00528
	ADH	0.00743	0.00223	0.00438	0.00805	0.00201	0.00528
$\Gamma = 0.2$	HNC	0.0203	0.00608	0.0120	0.0321	0.00757	0.0217
	DH	0.0243	0.00728	0.0143	0.0276	0.00603	0.0192
	ADH	0.0239	0.00716	0.0141	0.0273	0.00590	0.0191
$\Gamma = 0.5$	HNC	0.0894	0.0268	0.0527	0.170	0.0340	0.124
	DH	0.0494	0.0148	0.0292	0.0691	0.00470	0.0648
$\Gamma = 1$	HNC	0.239	0.0718	0.141	0.528	0.0841	0.422
	MHNC	0.241	0.0722	0.142	0.528	0.0842	0.422
$\Gamma = 2$	HNC	0.581	0.174	0.343	1.47	0.150	1.33
	MHNC	0.593	0.178	0.350	1.47	0.148	1.34

when Γ^{-1} is chosen for the upper limit of the integral, as before, one gets

$$\bar{\varphi}^s_{L,ij} = \tfrac{1}{2}\left(\frac{3}{\pi}\right)^{1/2}\Gamma^{5/2}\left[\ln\left(1+\frac{1}{3\Gamma^3}\right)-\frac{1}{1+3\Gamma^3}\right]c_{ij}. \tag{83}$$

For small values of Γ one finds, on a par with (78) and (82)

$$\bar{\varphi}^s_{L,ij} = \left(\frac{3}{\pi}\right)^{1/2}\Gamma^{5/2}[-\ln(\sqrt{3}\Gamma^{3/2})-\tfrac{1}{2}]c_{ij}. \tag{84}$$

The matrix elements of the composite kernel follow directly from those of its constituents, as given in the tables I and II. For $\Gamma \ll 1$ an approximate analytic formula is obtained from (78), (82) and (84):

$$\bar{\varphi}^s_{C,ij} = \left(\frac{3}{\pi}\right)^{1/2}\Gamma^{5/2}\left[-c_{ij}\ln(\sqrt{3}\Gamma^{3/2}) - d''_{ij}\right], \tag{85}$$

with $d''_{00} = 0.0688$, $d''_{01} = 0.3525$ and $d''_{11} = -0.1306$.

For comparison the matrix elements of the alternative kernel φ^s_{WB} (47) have been evaluated as well. This kernel is a modified form of the generalized Balescu–Guernsey–Lenard kernel φ^s_{BGL} (29); its matrix elements can be obtained from (67) by inserting an extra factor $-3(\Gamma/k^2)\,S(k)/[S(k)-1]$ in the integrand. Since this factor reduces to 1 in the Debye–Hückel approximation the matrix elements of the two kernels coincide in that case (see table II).

The self-diffusion coefficients that follow from the various memory kernels

Table III
Self-diffusion coefficients (in units $\omega_p a^2$) for moderately dense plasmas, with $0.1 < \Gamma < 2$, as found from a number of alternative memory kernels in the 1-Sonine- and 2-Sonine-polynomial approximation (first and second line of each entry, respectively)

		D_C	D_{BGL}	D_{WB}	D_B	D_L
$\Gamma = 0.1$	HNC	114.9	158.2	121.6	122.6	173.3
		121.5	173.1	134.8	134.4	204.5
	DH	115.6	124.2	124.2	124.4	134.4
		122.0	137.2	137.2	136.2	158.6
	ADH	114.1	124.3	124.3	122.7	134.6
		120.3	137.3	137.3	134.2	158.8
$\Gamma = 0.2$	HNC	30.1	43.4	31.2	32.9	49.3
		31.2	46.5	34.0	35.3	58.2
	DH	30.8	36.2	36.2	34.3	41.2
		31.7	38.9	38.9	36.8	48.6
	ADH	31.9	36.6	36.6	35.8	41.9
		32.5	39.2	39.2	37.8	49.5
$\Gamma = 0.5$	HNC	6.10	9.20	5.90	6.92	11.2
		6.16	9.53	6.24	7.22	13.2
	DH	6.91	14.5	14.5	7.99	20.2
		6.94	14.5	14.5	8.33	23.9
$\Gamma = 1$	HNC	2.11	3.22	1.90	2.49	4.18
		2.11	3.26	1.96	2.55	4.93
	MHNC	2.10	3.20	1.89	2.48	4.16
		2.10	3.25	1.96	2.53	4.91
$\Gamma = 2$	HNC	0.830	1.24	0.681	1.02	1.72
		0.833	1.25	0.689	1.03	2.03
	MHNC	0.815	1.22	0.680	1.00	1.69
		0.818	1.22	0.687	1.01	1.99

with the use of (57)–(59) have been collected in table III. All kernels predict that the self-diffusion coefficient diminishes rapidly with increasing Γ. In particular, for $\Gamma \ll 1$ one finds from (78), (82), (84) or (85) that D is proportional to $\Gamma^{-5/2}/(\ln \Gamma)$. Although the qualitative behaviour of the self-diffusion coefficient is the same for all kernels the numerical values for D are distinct, even for low values of Γ.

Let us consider first the self-diffusion coefficients D_C following from the use of the composite kernel which includes both the effects of close binary collisions and of collective interactions in the plasma. For $\Gamma = 0.1$ the values that follow by using the HNC pair correlation function differ by less than 1% from those obtained by applying the Debye–Hückel approximation (or its

crude form ADH). When Γ increases the differences become more pronounced; in particular, for $\Gamma = 0.5$ the Debye–Hückel approximation is no longer reliable. At $\Gamma = 1$ or 2 the modification of the hypernetted-chain equations proposed recently is found to lead to self-diffusion coefficients that do not differ significantly from the pure HNC results.

The use of higher Sonine polynomials in the evaluation of the self-diffusion coefficient on the basis of the composite kernel turns out to give rise to quickly converging results. The largest differences between $D^{(0)}$ and $D^{(1)}$ occur for $\Gamma = 0.1$. From the leading terms in (85) for $\Gamma \ll 1$ it follows that the first two approximations will eventually differ by a factor 1.18.

A comparison of the calculated self-diffusion coefficients with experimental data is possible only for $\Gamma = 1$, since most results of the molecular dynamics experiments refer to plasmas of a higher density[28,29]). The most recent experimental value[29]) for $\Gamma = 1$, *viz* $D = 2.05$, compares favourably with the result $D = 2.10$ found here.

The self-diffusion coefficient in moderately dense (and dense) plasmas has been studied previously on the basis of the generalized Balescu–Guernsey–Lenard kernel φ_{BGL} and its modified form φ_{WB}[6,7]). From the table it is seen that the self-diffusion coefficients that follow from the generalized BGL kernel are systematically too high by a factor of the order of 1.5. This peculiarity has been noted already in ref. 6. It was conjectured there that the inclusion of higher order Sonine polynomials might improve the results; the present calculation shows, however, that this is not the case. The discrepancy should be ascribed in fact to the incorrect treatment of the close binary collision in the BGL kernel. Another peculiar feature of the generalized Balescu–Guernsey–Lenard kernel is that the ensuing self-diffusion coefficients are rather sensitive to the use of the Debye–Hückel approximation, even for small Γ; apparently the application of a cutoff that is necessary to render the Debye–Hückel integral finite leads to a rather drastic change in D already for $\Gamma = 0.1$.

The values of the self-diffusion coefficient that follow from the modified kernel φ_{WB} are much nearer to those of the composite kernel. The convergence of the polynomial expansion turns out to be somewhat slower for the WB kernel. In particular, it is found that for $\Gamma = 0.1$ the lowest-order approximation is changed by more than 10% when a second Sonine polynomial is included. The resulting values are considerably higher in this case than those following from φ_{C}. For $\Gamma = 1$ the self-diffusion coefficient $D_{\mathrm{WB}} = 1.96$ as calculated here is a good approximation to the molecular-dynamics result $D = 2.05$, although the agreement seems to be somewhat less convincing than for the composite kernel. It should be remarked that in a recent review[30]) a value $D = 2.04$ is cited in connexion with the kernel φ_{WB}; the reason for the discrepancy is not clear.

The discussion of the results for the other two kernels, *viz.* the generalized Boltzmann and the generalized Landau kernels, can be brief. Neither of these yield quantitatively correct values of the self-diffusion coefficient for a moderately dense plasma, as a comparison with the molecular-dynamics result for $\Gamma = 1$ shows; the Boltzmann value is more than 20% too high, the Landau value even 140%. For a dilute plasma, with $\Gamma = 0.1$, the Boltzmann diffusion coefficient is still 10% higher than that of the composite kernel; the Landau-type kernel remains completely unsatisfactory even in that regime. The neglect of collective plasma interactions in the calculation of the self-diffusion coefficient is hence unjustified. (Of course both kernels eventually give correct values for D in the limit of a vanishing plasma parameter.)

The above discussion of the numerical results leads to the conclusion that a kinetic description of a moderately dense plasma yields reliable values for the self-diffusion coefficient if both the close binary collisions and the collective interactions in the plasma are taken into account. The composite kernel φ_C introduced in this paper takes care of these processes through a unification of generalized forms of the Boltzmann and Balescu–Guernsey–Lenard kernels. It has the additional advantage of guaranteeing the correct short-time behaviour of the time correlation function, since it satisfies the first-order sum rule by virtue of the well-established approximate validity of the hypernetted-chain equation for the static distribution functions in a plasma.

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