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SELF-DIFFUSION IN A DENSE MAGNETIZED PLASMA

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Self-diffusion through dense classical one-component plasmas in a uniform magnetic field is studied by means of renormalized kinetic theory. Extensions of the Landau and the Rostoker equations to plasmas of high density are derived. The coefficient of self-diffusion along the magnetic field is evaluated from the 1-Sonine approximation of the Landau kernel. The results show how the diffusion process is gradually impeded as the magnetic field strength increases.

1. Introduction

The dynamical properties of strongly coupled plasmas have been studied extensively in the past few years[1]). As a result of both computer simulations and theoretical investigations much is now known about the transport properties of these dense plasmas. Most of the results obtained so far refer to plasmas that are not situated in external electromagnetic fields. Recently, however, molecular dynamics simulations have been used to obtain information on the self-diffusion process through a strongly coupled plasma in a magnetic field[2]).

It is the purpose of this paper to give a kinetic description of self-diffusion in a dense magnetized plasma. To that end we shall apply the kinetic theory of dense fluids to a strongly coupled plasma in a magnetic field. The plasma screening effects will be incorporated through a renormalization of the interparticle potentials. In the case of an unmagnetized plasma this renormalized kinetic theory has led to results[3–5]) for the self-diffusion coefficient that compare favourably with the simulation data.

The kinetic equations that we shall derive in this paper can be considered as generalizations of well-known equations for a hot dilute magnetoplasma. As an example of the latter we mention the Landau equation for a magnetized plasma[6]), which is obtained by employing a weak-interaction approximation; in a previous paper[7]) we used this equation to calculate the self-diffusion coefficient in a dilute plasma as a function of the magnetic field. If dynamical screening effects are included in the Landau-type equation one arrives at the Rostoker equation[8]). In the following both equations will be generalized for dense plasmas.

As a model we shall consider the dense plasma to consist of a single component of charged particles in an inert uniform background of opposite charge[1]). The self-diffusion coefficient will be calculated from the time correlation function that describes the motion of a tagged particle. This time correlation function satisfies a kinetic equation the central quantity of which is a memory kernel that accounts for the interparticle interactions.

The paper is organized as follows. In section 2 the renormalized kinetic theory for magnetized dense plasmas will be developed. Subsequently, in section 3, generalizations of the Landau and the Rostoker memory kernels will be derived by introducing suitable approximations for the two-particle time correlation function that is contained in the memory kernel. In section 4, finally, numerical values for the self-diffusion coefficient will be presented.

2. Renormalized kinetic theory for a magnetized plasma

The time correlation function C^s, which describes the motion of a tagged particle through a magnetized plasma is defined by its Laplace transform as

$$C^s(\boldsymbol{rp}, \boldsymbol{r}'\boldsymbol{p}'; z) = -\mathrm{i} \int_0^\infty \mathrm{d}t\, \mathrm{e}^{\mathrm{i}zt} \langle \delta f^s(\boldsymbol{rp}; t) \delta f^s(\boldsymbol{r}'\boldsymbol{p}'; 0) \rangle , \tag{2.1}$$

with $\operatorname{Im} z > 0$. Here the brackets denote a canonical ensemble average. Furthermore the phase-space density fluctuation $\delta f^s = f^s - \langle f^s \rangle$ is given by

$$f^s(\boldsymbol{rp}; t) = \sqrt{N} \delta[\boldsymbol{r} - \boldsymbol{r}_s(t)] \delta[\boldsymbol{p} - \boldsymbol{p}_s(t)] , \tag{2.2}$$

with N the total number of particles and $\boldsymbol{r}_s(t)$, $\boldsymbol{p}_s(t)$ the position and momentum of the tagged particle at time t. In the following the symbol $\boldsymbol{x}$ will be used to denote a point $(\boldsymbol{r}, \boldsymbol{p})$ in phase space. The $(k+l)$-point time correlation functions $C^s_{k,l}(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_k, \boldsymbol{x}'_1, \ldots, \boldsymbol{x}'_l; z)$ for the tagged particle are defined in a way analogous to (2.1) (cf. (I.3)[5])). Likewise, the time correlation functions for arbitrary particles in the plasma are denoted by C_{kl} (the subscripts are omitted if $k = l = 1$).

The time correlation functions $C^s_{k,l}$ and $C_{k,l}$ will in general depend on the magnetic field, since the motion of the particles is influenced by the field. The static correlation functions $\tilde{C}^s_{k,l}$ and $\tilde{C}_{k,l}$, however, are the same for the unmagnetized and the magnetized plasma. This is a consequence of the theorem of Bohr and Van Leeuwen. In particular one has

$$\tilde{C}^s(\boldsymbol{x}, \boldsymbol{x}') = n f_0(p) \delta(\boldsymbol{x} - \boldsymbol{x}') , \tag{2.3}$$

$$\tilde{C}(\boldsymbol{x}, \boldsymbol{x}') = n f_0(p) \delta(\boldsymbol{x} - \boldsymbol{x}') + n^2 f_0(p) f_0(p') h(\boldsymbol{r} - \boldsymbol{r}') , \tag{2.4}$$

with $f_0(p)$ the normalized Maxwell–Boltzmann distribution function and

$h(\boldsymbol{r}) = g(\boldsymbol{r}) - 1$ the configurational pair correlation function of an unmagnetized plasma with the same density and temperature.

The dependence of C^s on the magnetic field becomes obvious when one writes down its kinetic equation

$$[z - L_0^B(\boldsymbol{x})]C^s(\boldsymbol{x}, \boldsymbol{x}'; z) - \int \mathrm{d}\boldsymbol{x}'' \, \varphi^s(\boldsymbol{x}, \boldsymbol{x}''; z) C^s(\boldsymbol{x}'', \boldsymbol{x}'; z) = \tilde{C}^s(\boldsymbol{x}, \boldsymbol{x}') . \tag{2.5}$$

Here L_0^B is the Liouville operator associated with the motion of a single charged particle, of charge e and mass m, in the uniform and stationary magnetic field $\boldsymbol{B}$

$$L_0^B(\boldsymbol{rp}) = -\frac{\mathrm{i}}{m}\boldsymbol{p} \cdot \nabla_{\boldsymbol{r}} - \mathrm{i}\omega_B(\boldsymbol{p} \wedge \hat{\boldsymbol{B}}) \cdot \nabla_{\boldsymbol{p}} , \tag{2.6}$$

where ω_B is the cyclotron frequency eB/mc and $\hat{\boldsymbol{B}}$ a unit vector in the direction of the field. The memory kernel φ^s in (2.5) describes the effect of interparticle interactions. It can be written in the form

$$\varphi^s(\boldsymbol{x}_1, \boldsymbol{x}_1'; z) n f_0(p_1') = -\int \mathrm{d}\boldsymbol{x}_2 \, \mathrm{d}\boldsymbol{x}_2' \, L_I(\boldsymbol{x}_1, \boldsymbol{x}_2) L_I(\boldsymbol{x}_1', \boldsymbol{x}_2') G_{2,2}^s(\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_1', \boldsymbol{x}_2'; z) , \tag{2.7}$$

with L_I the interaction operator

$$L_I(\boldsymbol{x}_1, \boldsymbol{x}_2) = \mathrm{i}[\nabla_{\boldsymbol{r}_1} v(\boldsymbol{r}_1 - \boldsymbol{r}_2)] \cdot (\nabla_{\boldsymbol{p}_1} - \nabla_{\boldsymbol{p}_2}) , \tag{2.8}$$

which contains the Coulomb potential $v(\boldsymbol{r}) = e^2/(4\pi r)$. The four-point function $G_{2,2}^s$ can be expressed[5]) in terms of the functions $C_{k,l}^s$ introduced above. An approximate form for $G_{2,2}^s$ may be found by solving, as in I, the kinetic equation for $G_{2,2}^s$ in the mean-field approximation. The kinetic kernel φ^s then becomes

$$\begin{aligned} \varphi^s(\boldsymbol{x}_1, \boldsymbol{x}_1'; z) n f_0(p_1') = -n^4 \int \mathrm{d}\boldsymbol{x}_2 \, \mathrm{d}\boldsymbol{x}_2' \, \tilde{L}_I(\boldsymbol{x}_1, \boldsymbol{x}_2) \\ \times \tilde{L}_I(\boldsymbol{x}_1', \boldsymbol{x}_2') f_0(p_1) f_0(p_2) g(\boldsymbol{r}_1 - \boldsymbol{r}_2) f_0(p_1') f_0(p_2') g(\boldsymbol{r}_1' - \boldsymbol{r}_2') \\ \times \bar{G}_{2,2}^s(\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_1', \boldsymbol{x}_2'; z) . \end{aligned} \tag{2.9}$$

The renormalized interaction operator

$$\tilde{L}_I(\boldsymbol{x}_1, \boldsymbol{x}_2) = -\mathrm{i}\beta^{-1}[\nabla_{\boldsymbol{r}_1} \log g(\boldsymbol{r}_1 - \boldsymbol{r}_2)] \cdot (\nabla_{\boldsymbol{p}_1} - \nabla_{\boldsymbol{p}_2}) \tag{2.10}$$

contains the effective interaction $v_{\mathrm{eff}}(\boldsymbol{r}) = -\beta^{-1} \log g(\boldsymbol{r}_1 - \boldsymbol{r}_2)$ with $\beta = 1/k_B T$. In the sequel we will not need the precise form of the reduced four-point function $\bar{G}_{2,2}^s$. At this point we merely note that it is an extension of the corresponding function for an unmagnetized plasma, as defined in (I.17).

3. Generalized Landau and Rostoker memory kernels for a magnetized plasma

The memory kernel (2.9) is basically determined by the reduced four-point function $\bar{G}^s_{2,2}$, which describes the dynamic correlations that build up if a pair of particles (the tagged particle and an arbitrary 'field' particle) move through the plasma. As $\bar{G}^s_{2,2}$ is too complicated we shall introduce an approximation so as to obtain a useful expression for the memory kernel (2.9). For an unmagnetized plasma we have shown[5]) that a generalized form of the Balescu–Guernsey–Lenard kernel is found if in the four-point function the correlations between the tagged particle and the field particles are disregarded. In this way the collective interactions in the plasma are taken into account; however, close binary collisions are then not treated adequately. In the present case of a magnetized plasma a similar approach may be followed. It will lead to a generalization of the Rostoker kernel.

The 'disconnected approximation' described above leads to the following form for the inverse of the four-point function $\bar{G}^s_{2,2}$:

$$[\bar{G}^s_{2,2}(\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}'_1, \boldsymbol{x}'_2; z)]^{-1} = n^2 f_0(p_1) f_0(p_2)\{[z - L^B_0(\boldsymbol{x}_1) - L^B_0(\boldsymbol{x}_2)]\delta(\boldsymbol{x}_2 - \boldsymbol{x}'_2) + nh(\boldsymbol{r}_2 - \boldsymbol{r}'_2) f_0(p'_2)[z - L^B_0(\boldsymbol{x}_1)]\}\delta(\boldsymbol{x}_1 - \boldsymbol{x}'_1) \tag{3.1}$$

(cf. (I.23)). An even more radical simplification that will lead to a Landau-type kernel results by neglecting the effects of static correlations between the field particles

$$[\bar{G}^s_{2,2}(\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}'_1, \boldsymbol{x}'_2; z)]^{-1} = n^2 f_0(p_1) f_0(p_2) \times [z - L^B_0(\boldsymbol{x}_1) - L^B_0(\boldsymbol{x}_2)]\delta(\boldsymbol{x}_1 - \boldsymbol{x}'_1)\delta(\boldsymbol{x}_2 - \boldsymbol{x}'_2). \tag{3.2}$$

In the following we shall derive the memory kernels that follow from (3.2) and (3.1), in that order.

To find the inverse of the right-hand side of (3.2) one starts by introducing spatial Fourier transforms in the usual way (see (I.24)). Then L^B_0 becomes

$$L^B_0(\boldsymbol{k}\boldsymbol{p}) = \frac{\boldsymbol{k}\cdot\boldsymbol{p}}{m} - \mathrm{i}\omega_B(\boldsymbol{p} \wedge \hat{\boldsymbol{B}})\cdot\nabla_{\boldsymbol{p}}. \tag{3.3}$$

In terms of this operator the inverse of (3.2) is given by a formal expression that reduces to (I.31) if the magnetic field is switched off:

$$\bar{G}^s_{2,2}(\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{q}, \boldsymbol{p}_1\boldsymbol{p}_2\boldsymbol{p}'_1\boldsymbol{p}'_2; z) = \frac{(2\pi)^3\delta(\boldsymbol{q})}{n^2 f_0(p_1) f_0(p_2)}[z - L^B_0(\boldsymbol{k}_1\boldsymbol{p}_1) - L^B_0(\boldsymbol{k}_2\boldsymbol{p}_2)]^{-1}\delta(\boldsymbol{p}_1 - \boldsymbol{p}'_1)\delta(\boldsymbol{p}_2 - \boldsymbol{p}'_2). \tag{3.4}$$

The inverse of the operator between brackets is evaluated in appendix A; from

(A.10) we get

$$\bar{G}^{s}_{2,2}(\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{q}, \boldsymbol{p}_1\boldsymbol{p}_2\boldsymbol{p}'_1\boldsymbol{p}'_2; z) = -\mathrm{i}\frac{(2\pi)^3\delta(\boldsymbol{q})}{n^2 f_0(p_1)f_0(p_2)}$$

$$\times \int_0^\infty \mathrm{d}t\, \mathrm{e}^{\mathrm{i}zt}\, \mathrm{e}^{-\mathrm{i}\boldsymbol{k}_1\cdot\boldsymbol{\alpha}_t\cdot\boldsymbol{p}_1/m - \mathrm{i}\boldsymbol{k}_2\cdot\boldsymbol{\alpha}_t\cdot\boldsymbol{p}_2/m}\delta(\boldsymbol{\gamma}_t\cdot\boldsymbol{p}_1 - \boldsymbol{p}'_1)\delta(\boldsymbol{\gamma}_t\cdot\boldsymbol{p}_2 - \boldsymbol{p}'_2)\,, \tag{3.5}$$

with $\boldsymbol{\alpha}_t$ and $\boldsymbol{\gamma}_t$ defined through

$$\boldsymbol{\alpha}_t\cdot\boldsymbol{p} = \boldsymbol{p}_{\|}t + \frac{\boldsymbol{p}_{\perp}}{\omega_B}\sin\omega_B t - \frac{\boldsymbol{p}_{\perp}\wedge\hat{\boldsymbol{B}}}{\omega_B}(1-\cos\omega_B t)\,, \tag{3.6}$$

$$\boldsymbol{\gamma}_t\cdot\boldsymbol{p} = \boldsymbol{p}_{\|} + \boldsymbol{p}_{\perp}\cos\omega_B t - \boldsymbol{p}_{\perp}\wedge\hat{\boldsymbol{B}}\sin\omega_B t\,. \tag{3.7}$$

Here $\boldsymbol{p}_{\|}$ and $\boldsymbol{p}_{\perp}$ are the longitudinal and the transverse components of $\boldsymbol{p}$ with respect to the magnetic field, respectively.

The Fourier-transformed version of the memory kernel (2.9) contains the integral over $\boldsymbol{p}_2$ and $\boldsymbol{p}'_2$ of $\bar{G}^{s}_{2,2}f_0(p_2)f_0(p'_2)$. The integration over $\boldsymbol{p}'_2$ can be performed trivially, while the integration over $\boldsymbol{p}_2$ leads to an integral of the form

$$F_B(\boldsymbol{k}, t) = \int \mathrm{d}\boldsymbol{p}\, \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{\alpha}_t\cdot\boldsymbol{p}/m} f_0(p)$$

$$= \exp[-k_{\|}^2 t^2/(2m\beta) - k_{\perp}^2(1-\cos\omega_B t)/(m\beta\omega_B^2)]\,. \tag{3.8}$$

In the following we shall also need the Laplace transform $F_B(\boldsymbol{k}, z) = -\mathrm{i}\int_0^\infty \mathrm{d}t\, \exp(\mathrm{i}zt)F_B(\boldsymbol{k}, t)$. In the absence of a magnetic field one has $\boldsymbol{\alpha}_t = \boldsymbol{U}t$ and hence

$$F(\boldsymbol{k}, z) = \int \mathrm{d}\boldsymbol{p}\frac{f_0(p)}{z - \boldsymbol{k}\cdot\boldsymbol{p}/m} = \frac{1}{z}\left[1 - W\left(\sqrt{m\beta}\,\frac{z}{k}\right)\right], \tag{3.9}$$

with W the plasma function[9]). For $B \neq 0$ we may again express $F_B(\boldsymbol{k}, z)$ in the plasma function by using the identity[10])

$$\mathrm{e}^{z\cos t} = \sum_{n=-\infty}^{\infty} I_n(z)\,\mathrm{e}^{\mathrm{i}nt}\,, \tag{3.10}$$

with I_n the modified Bessel function, in the last member of (3.8). Then one gets[9])

$$F_B(\boldsymbol{k}, z) = \sum_n \frac{1}{z - n\omega_B}\left[1 - W\left(\sqrt{m\beta}\,\frac{z - n\omega_B}{|k_{\|}|}\right)\right]\Lambda_n\left(\frac{k_{\perp}^2}{m\beta\omega_B^2}\right), \tag{3.11}$$

with $\Lambda_n(x) = \mathrm{e}^{-x}I_n(x)$.

Combining (3.5) and (3.8) we have found now

$$\int \mathrm{d}\boldsymbol{p}_2\, \mathrm{d}\boldsymbol{p}_2'\, \bar{G}^s_{2,2}(\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{q}, \boldsymbol{p}_1\boldsymbol{p}_2\boldsymbol{p}_1'\boldsymbol{p}_2'; z)n^2 f_0(p_2) f_0(p_2')$$
$$= -\mathrm{i}\frac{(2\pi)^3\delta(\boldsymbol{q})}{f_0(p_1)} \int_0^\infty \mathrm{d}t\, \mathrm{e}^{\mathrm{i}zt}\, \mathrm{e}^{-\mathrm{i}\boldsymbol{k}_1\cdot\boldsymbol{\alpha}_t\cdot\boldsymbol{p}_1/m} F_B(\boldsymbol{k}_2, t)\delta(\gamma_t\cdot\boldsymbol{p}_1 - \boldsymbol{p}_1') \,. \tag{3.12}$$

Insertion of (3.12) in the Fourier transform of (2.9) finally leads to the following expression for the memory kernel:

$$\varphi^s_{\mathrm{L}}(\boldsymbol{k}\boldsymbol{p}\boldsymbol{p}'; z) n f_0(p') = -\mathrm{i}\frac{n^2}{\beta^2}\int \frac{\mathrm{d}\boldsymbol{q}}{(2\pi)^3}[h(q)]^2 \boldsymbol{q}\cdot\boldsymbol{\nabla}_p \boldsymbol{q}\cdot\boldsymbol{\nabla}_{p'}$$
$$\times \left[f_0(p) \int_0^\infty \mathrm{d}t\, \mathrm{e}^{\mathrm{i}zt - \mathrm{i}(\boldsymbol{k}-\boldsymbol{q})\cdot\boldsymbol{\alpha}_t\cdot\boldsymbol{p}/m} F_B(\boldsymbol{q}, t)\delta(\gamma_t\cdot\boldsymbol{p} - \boldsymbol{p}')\right]. \tag{3.13}$$

For $B \to 0$ one easily recovers the Landau kernel given previously (cf. (I.32)). The Landau-type kernel found here is the extension of that result to the case of a magnetized dense plasma.

To derive a Balescu–Guernsey–Lenard type memory kernel for a magnetized plasma we start from (3.1) instead of (3.2). By inspection of the corresponding expression (I.25) for the unmagnetized plasma we immediately write down the inverse of (3.1)

$$\bar{G}^s_{2,2}(\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{q}, \boldsymbol{p}_1\boldsymbol{p}_1'\boldsymbol{p}_2\boldsymbol{p}_2'; z) = \frac{(2\pi)^3\delta(\boldsymbol{q})}{n f_0(p_1)}[z - L_0^B(\boldsymbol{k}_1\boldsymbol{p}_1) - L_0^B(\boldsymbol{k}_2\boldsymbol{p}_2)]^{-1}$$
$$\times\left\{\frac{\delta(\boldsymbol{p}_1 - \boldsymbol{p}_1')\delta(\boldsymbol{p}_2 - \boldsymbol{p}_2')}{n f_0(p_2)} - c(k_2)[z - L_0^B(\boldsymbol{k}_1\boldsymbol{p}_1)][\epsilon_B(\boldsymbol{k}_2, z - L_0^B(\boldsymbol{k}_1\boldsymbol{p}_1)]^{-1}\right.$$
$$\left.\times [z - L_0^B(\boldsymbol{k}_1\boldsymbol{p}_1) - L_0^B(\boldsymbol{k}_2, \boldsymbol{p}_2')]^{-1}\delta(\boldsymbol{p}_1 - \boldsymbol{p}_1')\right\}, \tag{3.14}$$

with $c(k) = h(k)/[1 + nh(k)]$ the direct correlation function and

$$\epsilon_B(\boldsymbol{k}, z) = 1 + nc(k)[zF_B(\boldsymbol{k}, z) - 1]\,, \tag{3.15}$$

the dielectric function of the magnetized plasma. The expression (3.14) is rather formal. Using (A.9) and (A.10) one obtains a more explicit expression,

$$\bar{G}^s_{2,2}(\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{q}, \boldsymbol{p}_1\boldsymbol{p}_1'\boldsymbol{p}_2\boldsymbol{p}_2'; z) = -\mathrm{i}\frac{(2\pi)^3\delta(\boldsymbol{q})}{n f_0(p_1)}\int_0^\infty \mathrm{d}t\, \mathrm{e}^{\mathrm{i}zt - \mathrm{i}\boldsymbol{k}_1\cdot\boldsymbol{\alpha}_t\cdot\boldsymbol{p}_1/m}$$
$$\times \left[\frac{\mathrm{e}^{-\mathrm{i}\boldsymbol{k}_2\cdot\boldsymbol{\alpha}_t\cdot\boldsymbol{p}_2/m}}{n f_0(p_2)}\delta(\gamma_t\cdot\boldsymbol{p}_2 - \boldsymbol{p}_2') + c(k_2)\int_0^t \mathrm{d}t' \int_0^{t'} \mathrm{d}t''\right.$$

$$\times \frac{\mathrm{i}}{2\pi} \int_{-\infty+\mathrm{i}0}^{\infty+\mathrm{i}0} \mathrm{d}z' \frac{z'}{\epsilon_B(\boldsymbol{k}_2, z')} \exp(-\mathrm{i}z't'' - \mathrm{i}\boldsymbol{k}_2 \cdot \boldsymbol{\alpha}_{t-t'} \cdot \boldsymbol{p}_2/m$$

$$+ \mathrm{i}\boldsymbol{k}_2 \cdot \boldsymbol{\alpha}_{-t'+t''} \cdot \boldsymbol{p}_2'/m) \Bigg] \delta(\gamma_t \cdot \boldsymbol{p}_1 - \boldsymbol{p}_1') . \tag{3.16}$$

To evaluate the memory kernel we start by multiplying this expression by $n^2 f_0(p_2) f_0(p_2')$ and integrate over $\boldsymbol{p}_2$ and $\boldsymbol{p}_2'$, as before. The first term within the brackets then leads again to (3.12). In the second term we can likewise introduce $F_B(\boldsymbol{k}, t)$ through (3.8). The time integrals can then be performed consecutively. As a result this term gives rise to the following expression:

$$\frac{\mathrm{i}(2\pi)^3 \delta(\boldsymbol{q}) n c(k_2)}{f_0(p_1)} \int_0^\infty \mathrm{d}t\, \mathrm{e}^{\mathrm{i}zt - \mathrm{i}\boldsymbol{k}_1 \cdot \boldsymbol{\alpha}_t \cdot \boldsymbol{p}_1/m}$$

$$\times \frac{\mathrm{i}}{2\pi} \int_{-\infty+\mathrm{i}0}^{\infty+\mathrm{i}0} \mathrm{d}z' \frac{z'[F_B(\boldsymbol{k}_2, z')]^2 \mathrm{e}^{-\mathrm{i}z't}}{\epsilon_B(\boldsymbol{k}_2, z')} \delta(\gamma_t \cdot \boldsymbol{p}_1 - \boldsymbol{p}_1') . \tag{3.17}$$

With the use of (3.15) the sum of (3.12) and (3.17) may be written as

$$\int \mathrm{d}\boldsymbol{p}_2\, \mathrm{d}\boldsymbol{p}_2' \bar{G}^s_{2,2}(\boldsymbol{k}_1 \boldsymbol{k}_2 \boldsymbol{q}, \boldsymbol{p}_1 \boldsymbol{p}_1' \boldsymbol{p}_2 \boldsymbol{p}_2'; z) n^2 f_0(p_2) f_0(p_2')$$

$$= \frac{-\mathrm{i}\, (2\pi)^3 \delta(\boldsymbol{q})}{f_0(p_1)} [1 - nc(k_2)] \int_0^\infty \mathrm{d}t\, \mathrm{e}^{\mathrm{i}zt}\, \mathrm{e}^{-\mathrm{i}\boldsymbol{k}_1 \cdot \boldsymbol{\alpha}_t \cdot \boldsymbol{p}_1/m}$$

$$\times \frac{\mathrm{i}}{2\pi} \int_{-\infty+\mathrm{i}0}^{\infty+\mathrm{i}0} \mathrm{d}z' \frac{F_B(\boldsymbol{k}_2, z')}{\epsilon_B(\boldsymbol{k}_2, z')} \mathrm{e}^{-\mathrm{i}z't} \delta(\gamma_t \cdot \boldsymbol{p}_1 - \boldsymbol{p}_1') . \tag{3.18}$$

The ensuing expression for the memory kernel then becomes

$$\varphi^s_{\mathrm{R}}(\boldsymbol{k}\boldsymbol{p}\boldsymbol{p}'; z) n f_0(p') = -\mathrm{i} \frac{n^2}{\beta^2} \int \frac{\mathrm{d}\boldsymbol{q}}{(2\pi)^3} c(q) h(q) \boldsymbol{q} \cdot \nabla_{\boldsymbol{p}} \boldsymbol{q} \cdot \nabla_{\boldsymbol{p}'}$$

$$\times \left[f_0(p) \int_0^\infty \mathrm{d}t\, \mathrm{e}^{\mathrm{i}zt - \mathrm{i}(\boldsymbol{k}-\boldsymbol{q}) \cdot \boldsymbol{\alpha}_t \cdot \boldsymbol{p}/m} \frac{\mathrm{i}}{2\pi} \int_{-\infty+\mathrm{i}0}^{\infty+\mathrm{i}0} \mathrm{d}z' \frac{F_B(\boldsymbol{q}, z')}{\epsilon_B(\boldsymbol{q}, z')} \mathrm{e}^{-\mathrm{i}z't} \delta(\gamma_t \cdot \boldsymbol{p} - \boldsymbol{p}') \right] . \tag{3.19}$$

A comparison of this kernel with the Landau kernel (3.13) shows that, apart from a minor change in the static correlation functions, the main feature of (3.19) is the occurrence of the dynamic screening factor ϵ_B, which is characteristic for a memory kernel of the Balescu–Guernsey–Lenard (BGL)–type. If the magnetic field is removed (3.19) indeed reduces to (I.28), as can be seen in the following way. If $B = 0$ the time integral in (3.19) is trivial. The integrand of the z'-integral then acquires a pole at $z' = z - (\boldsymbol{k} - \boldsymbol{q})\cdot\boldsymbol{p}/m$. Carrying out the z'-integration one recovers (I.28). Since for a dilute plasma the generalization of the BGL-equation to the magnetized case is the Rostoker equation[8]) one may name (3.19) the generalized Rostoker kernel for a dense magnetized plasma.

The time correlation function C^s for a tagged particle in a magnetized plasma, and hence the memory kernel φ^s, possesses several symmetries that are a consequence of the space-time invariances of the Hamiltonian. In particular, parity invariance and the invariance under the combined effect of time translation and time reversal imply that φ^s should satisfy the relations

$$\varphi^s(\boldsymbol{k}, \boldsymbol{p}, \boldsymbol{p}'; z, \boldsymbol{B}) = \varphi^s(-\boldsymbol{k}, -\boldsymbol{p}, -\boldsymbol{p}'; z, \boldsymbol{B}), \tag{3.20}$$

$$\varphi^s(\boldsymbol{k}, \boldsymbol{p}, \boldsymbol{p}'; z, \boldsymbol{B}) f_0(p') = \varphi^s(-\boldsymbol{k}, -\boldsymbol{p}', -\boldsymbol{p}; z, -\boldsymbol{B}) f_0(p), \tag{3.21}$$

where we inserted explicitly the dependence of φ^s on $\boldsymbol{B}$. Furthermore, since the correlation functions are real we require

$$\varphi^s(\boldsymbol{k}, \boldsymbol{p}, \boldsymbol{p}'; z, \boldsymbol{B}) = -[\varphi^s(-\boldsymbol{k}, \boldsymbol{p}, \boldsymbol{p}'; -z^*, \boldsymbol{B})]^* . \tag{3.22}$$

These relations are indeed satisfied by the Landau and the Rostoker kernels (3.13) and (3.19). The proof of (3.20) for these kernels is straightforward. To prove (3.21) we need the identities

$$\boldsymbol{\alpha}_t(-\boldsymbol{B}) = \boldsymbol{\alpha}_t(\boldsymbol{B})\cdot\boldsymbol{\gamma}_{-t}(\boldsymbol{B}), \tag{3.23}$$

$$\boldsymbol{\gamma}_t(-\boldsymbol{B}) = \boldsymbol{\gamma}_{-t}(\boldsymbol{B}), \tag{3.24}$$

which follow directly from the definitions (3.6) and (3.7). The relations

$$F_B(\boldsymbol{q}, z) = -[F_B(\boldsymbol{q}, -z^*)]^* , \tag{3.25}$$

$$\epsilon_B(\boldsymbol{q}, z) = [\epsilon_B(\boldsymbol{q}, -z^*)]^* \tag{3.26}$$

are used in the proof of (3.22).

The conservation of the tagged particle number leads to the identity

$$\int \mathrm{d}\boldsymbol{p}\, \varphi^s(\boldsymbol{k}\boldsymbol{p}\boldsymbol{p}'; z) = 0 , \tag{3.27}$$

which is immediately verified for φ^s_{L} and φ^s_{R}.

The short-time behaviour of the time correlation function leads to sum rules the first of which is[5])

$$\lim_{z\to\infty} z\varphi^s(\boldsymbol{k}\boldsymbol{p}\boldsymbol{p}'; z) n f_0(p') = -\frac{n^2e^2}{3\beta}\int \frac{\mathrm{d}\boldsymbol{q}}{(2\pi)^3} h(q) \nabla_{\boldsymbol{p}}\cdot\nabla_{\boldsymbol{p}'} f_0(p)\delta(\boldsymbol{p} - \boldsymbol{p}') . \tag{3.28}$$

Neither the Landau nor the Rostoker memory kernel fulfils this sum rule. In fact one has

$$\lim_{z\to\infty} z\varphi^{s}_{L}(\boldsymbol{kpp}'; z)nf_0(p') = \frac{n^2}{3\beta}\int \frac{\mathrm{d}\boldsymbol{q}}{(2\pi)^3} q^2[h(q)]^2\nabla_{\boldsymbol{p}}\cdot\nabla_{\boldsymbol{p}'} f_0(p)\delta(\boldsymbol{p}-\boldsymbol{p}'), \tag{3.29}$$

$$\lim_{z\to\infty} z\varphi^{s}_{R}(\boldsymbol{kpp}'; z)nf_0(p') = \frac{n^2}{3\beta^2}\int \frac{\mathrm{d}\boldsymbol{q}}{(2\pi)^3} q^2 c(q)h(q)\nabla_{\boldsymbol{p}}\cdot\nabla_{\boldsymbol{p}'} f_0(p)\delta(\boldsymbol{p}-\boldsymbol{p}'). \tag{3.30}$$

Hence it must be concluded that neither the generalized Landau nor the generalized Rostoker memory kernel will lead to time correlation functions with the correct behaviour for small t. In the case of a vanishing magnetic field the same difficulty was dealt with by considering a composite kernel in which the Landau and BGL kernels contribute on a par with a Boltzmann-type memory kernel that takes account of close binary collisions[5]). However, since there is no explicit expression available for the scattering cross-section of charged particles in a magnetic field, the Boltzmann-type kernel for a magnetized plasma is rather unwieldy. Therefore in the present case no use will be made of a composite kernel.

An alternative approach[4,11]) that leads to memory kernels satisfying the sum rule (3.28) starts by writing the formal expression (2.9) for the memory kernel in a slightly different way. By replacing one of the renormalized operators $\tilde{L}_I$ by the bare operator L_I and changing $\bar{G}^{s}_{2,2}$ correspondingly one finds along similar lines as above modified versions of the Landau and the Rostoker memory kernels. The modified Landau kernel is obtained from (3.13) by replacing one of the factors $h(q)$ by $-\beta v(q)$, so that one gets

$$\varphi^{s}_{L'}(\boldsymbol{kpp}'; z)nf_0(p') = \frac{\mathrm{i}n^2}{\beta}\int \frac{\mathrm{d}\boldsymbol{q}}{(2\pi)^3} h(q)v(q)\boldsymbol{q}\cdot\nabla_{\boldsymbol{p}}\boldsymbol{q}\cdot\nabla_{\boldsymbol{p}'}$$
$$\times\left[f_0(p)\int_0^\infty \mathrm{d}t\, \mathrm{e}^{\mathrm{i}zt-\mathrm{i}(\boldsymbol{k}-\boldsymbol{q})\cdot\boldsymbol{\alpha}_t\cdot\boldsymbol{p}/m}F_B(\boldsymbol{q},t)\delta(\boldsymbol{\gamma}_t\cdot\boldsymbol{p}-\boldsymbol{p}')\right]. \tag{3.31}$$

The modified version of the Rostoker kernel follows from (3.19) by the substitution $c(q)\to-\beta v(q)$,

$$\varphi^{s}_{R'}(\boldsymbol{kpp}'; z)nf_0(p') = \mathrm{i}\frac{n^2}{\beta}\int \frac{d\boldsymbol{q}}{(2\pi)^3} h(q)v(q)\boldsymbol{q}\cdot\nabla_{\boldsymbol{p}}\boldsymbol{q}\cdot\nabla_{\boldsymbol{p}'}$$
$$\times\left[f_0(p)\int_0^\infty \mathrm{d}t\, \mathrm{e}^{\mathrm{i}zt-\mathrm{i}(\boldsymbol{k}-\boldsymbol{q})\cdot\boldsymbol{\alpha}_t\cdot\boldsymbol{p}/m}\frac{\mathrm{i}}{2\pi}\int_{-\infty+\mathrm{i}0}^{\infty+\mathrm{i}0}\mathrm{d}z'\frac{F_B(\boldsymbol{q},z')}{\epsilon_B(\boldsymbol{q},z')}\mathrm{e}^{-\mathrm{i}z't}\delta(\boldsymbol{\gamma}_t\cdot\boldsymbol{p}-\boldsymbol{p}')\right]. \tag{3.32}$$

Both (3.31) and (3.32) satisfy the sum rule (3.28), so that the correct short-time behaviour of C^s is guaranteed, if these kernels are used in the kinetic equation.

4. Evaluation of the longitudinal self-diffusion coefficient from the Landau and the modified Landau kernel

The coefficient of diffusion of a tagged particle through the magnetized plasma follows directly once the time correlation function C^s is known. Here we shall concentrate on the self-diffusion parallel to the magnetic field. The corresponding longitudinal diffusion coefficient is given by the Green–Kubo relation

$$D_\parallel = \frac{\mathrm{i}}{m^2 n} \lim_{z\to \mathrm{i}0} \int \mathrm{d}\boldsymbol{p}\, \mathrm{d}\boldsymbol{p}' p_\parallel C^s(\boldsymbol{k}=0, \boldsymbol{pp}'; z) p'_\parallel . \tag{4.1}$$

The time correlation function has to be determined from the kinetic equation (2.5) with one of the kernels derived in the preceding section. For simplicity we shall retain only the static screening effects; hence only the Landau kernel (3.13) and its modified version (3.31) will be considered. Upon substitution of the kernel the kinetic equation (2.5) becomes an integral equation in the momenta. It may be transformed into an infinite set of algebraic equations by introducing a complete set of functions in momentum space, as in paper I. It should be remarked here that the coupled equations that determine the longitudinal matrix element of C^s in (4.1) do not contain the B-dependent part of the Liouville operator L_0^B. When the equations are truncated in the usual way one finds in the 1-Sonine approximation

$$1/D_\parallel = \mathrm{i}\beta^2 \lim_{z\to \mathrm{i}0} \int \mathrm{d}\boldsymbol{p}\, \mathrm{d}\boldsymbol{p}' p_\parallel \varphi^s(\boldsymbol{k}=0, \boldsymbol{pp}'; z) p'_\parallel f_0(p') . \tag{4.2}$$

Inserting the Landau kernel (3.13) and performing the integrations over the momenta we get

$$1/D_{\parallel,\mathrm{L}} = n \int \frac{\mathrm{d}\boldsymbol{q}}{(2\pi)^3} [h(q)]^2 q_\parallel^2 \int_0^\infty \mathrm{d}s\, [F_B(\boldsymbol{q}, s)]^2 , \tag{4.3}$$

or, upon introducing the dimensionless variables $\boldsymbol{x} = \boldsymbol{q}/k_\mathrm{D}$ and $t = \omega_\mathrm{p} s$ (with k_D the inverse Debye length and ω_p the plasma frequency)

$$1/D_{\parallel,\mathrm{L}} = \frac{1}{\omega_\mathrm{p} a^2} \frac{2\Gamma^{5/2} 3^{3/2}}{\pi} \int_0^\infty \mathrm{d}x\, x^4 [1 - S(x)]^2 \int_0^1 \mathrm{d}z\, z^2 \int_0^\infty \mathrm{d}t\, \mathrm{e}^{-x^2 u - x^2 z^2 v} . \tag{4.4}$$

Here we employed the integration variable $z = \hat{\boldsymbol{x}} \cdot \hat{\boldsymbol{B}}$ and the abbreviations $u = 2b^{-2}(1 - \cos bt)$, $v = t^2 - u$, with $b = \omega_B/\omega_\mathrm{p}$ the dimensionless field strength.

Furthermore we introduced the static structure factor $S(x) = 1 + nh(x)$ and used the definitions for the ion radius $a = (3/4\pi n)^{1/3}$ and for the plasma coupling constant $\Gamma = \frac{1}{3}a^2k_D^2$.

For small values of Γ the structure factor $S(x)$ may be replaced by its Debye–Hückel form $x^2/(1+x^2)$. Then (4.4) reduces to the weak-coupling result evaluated in a previous paper[7]). In that case the integral over the wave vector is divergent for large x. This divergence is remedied in the usual way by imposing a cut-off at a wave vector corresponding to the inverse Landau length. One of the virtues of (4.4) is that it is convergent as it stands; even for small Γ the structure factor approaches 1 (as $x \to \infty$) more rapidly than its Debye–Hückel counterpart.

When the magnetic field is switched off, the integrations over t and z in (4.4) are easily performed. One then recovers the diffusion coefficient in the Landau approximation, which was investigated in paper I.

An alternative form of (4.4) is obtained by performing the integration over z, with the help of (II.3.2). Then we get

$$1/D_{\|,\mathrm{L}} = \frac{1}{\omega_p a^2}\Gamma^{5/2}\sqrt{\frac{3}{\pi}}\int_0^\infty \mathrm{d}x\, x^3[1-S(x)]^2\left[1+\frac{x}{b}K\left(\frac{x}{b}\right)\right], \tag{4.5}$$

where

$$K(x) = \frac{4}{5\sqrt{\pi}}\int_0^\infty \mathrm{d}t\, \mathrm{e}^{-t^2x^2} w\,{}_1F_1(1,\tfrac{7}{2},w), \tag{4.6}$$

with $w = [t^2 - 2(1-\cos t)]x^2$.

If the modified version (3.19) of the Landau kernel is used in the formal expression (4.2) for the inverse self-diffusion coefficient, a result similar to (4.5), but with a factor $[1-S(x)]/x^2$ instead of $[1-S(x)]^2$, is found.

In the Debye–Hückel approximation the expression (4.5) may be simplified further. Imposing an upper cut-off at $X = 1/\sqrt{3}\Gamma^{3/2}$ one finds then[7])

$$1/D_{\|,\mathrm{L}} = \frac{1}{\omega_p a^2}\Gamma^{5/2}\sqrt{\frac{3}{\pi}}\,[-\log(\sqrt{3}\Gamma^{3/2}) - \tfrac{1}{2} + J_\mathrm{L}(b,\Gamma)], \tag{4.7}$$

with

$$J_\mathrm{L}(b,\Gamma) = \int_0^{X/b} \mathrm{d}x\, \frac{x^4}{(b^{-2}+x^2)^2}K(x). \tag{4.8}$$

Likewise, the modified Landau kernel then leads to the formula

$$1/D_{\|,\mathrm{L'}} = \frac{1}{\omega_p a^2}\Gamma^{5/2}\sqrt{\frac{3}{\pi}}\,[-\log(\sqrt{3}\Gamma^{3/2}) + J_\mathrm{L'}(b,\Gamma)], \tag{4.9}$$

with

$$J_{L'}(b,\Gamma)=\int_0^{X/b}\mathrm{d}x\,\frac{x^2}{b^{-2}+x^2}\,K(x)\,. \tag{4.10}$$

The asymptotic forms of J_L for small and for large values of b have been given in paper II. The corresponding formulae for $J_{L'}$ are derived in appendix B.

The numerical evaluation of the self-diffusion coefficient is carried out with the use of the methods described in papers I and II. The integral $K(x)$ is calculated conveniently by dividing the integration interval in finite subintervals of length π and 2π. The structure factor is obtained by solving the hypernetted-chain equation, which yields a fair approximation for the static correlation functions of a dense plasma.

Since we are interested in the effects of the magnetic field on the diffusion process, the numerical results for $D_\parallel$ are presented here by giving the ratio

$$R_\parallel(b,\Gamma)=\frac{D_\parallel(b,\Gamma)}{D_\parallel(0,\Gamma)} \tag{4.11}$$

of the longitudinal self-diffusion coefficients in the presence and in the absence of the magnetic field. In tables I and II the results for $R_\parallel$ that follow by using the 1-Sonine approximation for the Landau and the modified Landau kinetic equations, respectively, are given for various values of b and Γ. Although the self-diffusion coefficient $D_\parallel$ depends strongly on the choice of the memory kernel, in particular for $\Gamma \gg 1$, it is found that the reduced self-diffusion coefficient $R_\parallel$, is rather insensitive to this choice; for $\Gamma \leq 10$ the two alternatives for $R_\parallel$ differ by less than 10%.

TABLE I

The reduced longitudinal self-diffusion coefficient $R_\parallel(b,\Gamma)$, as found from the Landau memory kernel φ_L in the 1-Sonine approximation

b \ Γ	0.1	0.2	0.5	1	2	5	10
0.1	1.000	1.000	1.000	1.000	0.999	0.999	0.998
0.2	1.000	1.000	0.999	0.998	0.997	0.994	0.989
0.5	0.998	0.996	0.993	0.988	0.977	0.951	0.920
1	0.990	0.984	0.969	0.946	0.909	0.840	0.795
2	0.961	0.942	0.897	0.844	0.785	0.729	0.709
5	0.876	0.832	0.761	0.715	0.690	0.678	0.674
10	0.799	0.751	0.699	0.680	0.673	0.670	0.669
20	0.737	0.700	0.676	0.670	0.668	0.667	0.667
50	0.689	0.674	0.668	0.667	0.667	0.667	0.667
100	0.674	0.669	0.667	0.667	0.667	0.667	0.667

TABLE II
The reduced longitudinal self-diffusion coefficient $R_{\|}(b, \Gamma)$, as found from the modified Landau memory kernel $\varphi_{L'}$ in the 1-Sonine approximation

b \ Γ	0.1	0.2	0.5	1	2	5	10
0.1	1.000	1.000	0.999	0.998	0.997	0.993	0.988
0.2	0.999	0.998	0.996	0.993	0.989	0.977	0.960
0.5	0.991	0.988	0.980	0.968	0.949	0.903	0.848
1	0.975	0.965	0.943	0.914	0.870	0.789	0.727
2	0.939	0.918	0.873	0.823	0.764	0.699	0.677
5	0.864	0.826	0.762	0.714	0.683	0.671	0.668
10	0.802	0.760	0.705	0.679	0.670	0.668	0.667
20	0.750	0.712	0.678	0.669	0.668	0.667	0.667
50	0.701	0.679	0.668	0.667	0.667	0.667	0.667
100	0.681	0.670	0.667	0.667	0.667	0.667	0.667

From the tables, or alternatively from figs. 1 and 2, it is seen that the diffusion process along the magnetic field is gradually impeded as the field strength increases. This effect becomes more prominent at higher values of the coupling parameter Γ. For strong magnetic fields $R_{\|}$ reaches an asymptotic value

$$\lim_{b\to\infty} R_{\|}(b, \Gamma) = \tfrac{2}{3}, \tag{4.12}$$

independent of Γ. This result, which we have found already in paper II for hot dilute plasmas, can easily be proved analytically from (4.5) by employing the

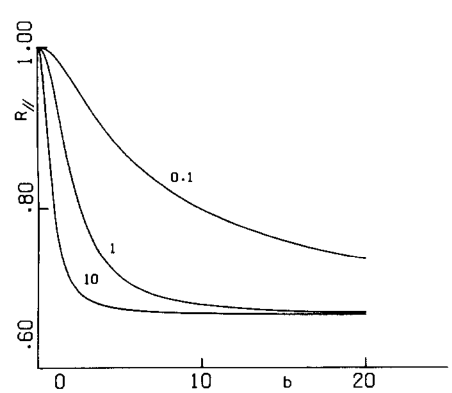

Fig. 1. $R_{\|}(b, \Gamma)$ for $\Gamma = 0.1$, 1 and 10, as found from the Landau kernel.

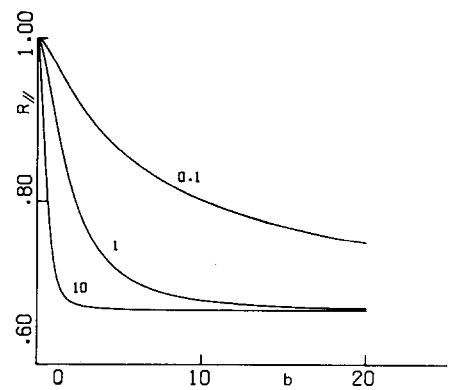

Fig. 2. $R_{\parallel}(b, \Gamma)$ for $\Gamma = 0.1$, 1 and 10, as found from the modified Landau kernel.

asymptotic formulae

$$\lim_{x\to 0} x K(x) = \tfrac{1}{2}, \qquad \lim_{x\to\infty} x K(x) = 0, \tag{4.13}$$

which follow from the definition (4.6)[7].

Recently the self-diffusion coefficient in a magnetized plasma has been determined for a few values of Γ and b with the help of molecular dynamics[2]. The experimental data show the same qualitative features as described above. In particular, it has been found with these simulations that the longitudinal diffusion process is indeed impeded by the magnetic field, at least for strongly coupled plasmas. The theoretical explanation of this effect, which is overlooked in a simple model based on a Gaussian memory function[2], is one of the main results of this paper.

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Appendix A

The streaming operator in a magnetic field

In sections 2 and 3 we used the streaming operator $L_0^B(\boldsymbol{kp})$ of a particle in a magnetic field, which is defined as

$$L_0^B(\boldsymbol{kp}) = \frac{\boldsymbol{k}\cdot\boldsymbol{p}}{m} - \mathrm{i}\omega_B(\boldsymbol{p} \wedge \hat{\boldsymbol{B}})\cdot\nabla_p . \tag{A.1}$$

The action of $\exp(-\mathrm{i}L_0^B t)$ on a function $f(\boldsymbol{p})$ of the momenta is given by the identity

$$\mathrm{e}^{-\mathrm{i}L_0^B(\boldsymbol{kp})t} f(\boldsymbol{p}) = \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{\alpha}_t\cdot\boldsymbol{p}/m} f(\boldsymbol{\gamma}_t\cdot\boldsymbol{p}) , \tag{A.2}$$

with the abbreviations (3.6) and (3.7). The proof of (A.2) follows by differentiating both sides with respect to t and making use of the ancillary relations

$$\frac{\mathrm{d}}{\mathrm{d}t}(\boldsymbol{\alpha}_t\cdot\boldsymbol{p}) = \boldsymbol{\gamma}_t\cdot\boldsymbol{p} , \tag{A.3}$$

and

$$\boldsymbol{\gamma}_t\cdot\boldsymbol{p} - \boldsymbol{p} = -\omega_B(\boldsymbol{p} \wedge \hat{\boldsymbol{B}})\cdot\nabla_p(\boldsymbol{\alpha}_t\cdot\boldsymbol{p}) , \tag{A.4}$$

which imply

$$\frac{\mathrm{d}}{\mathrm{d}t}(\boldsymbol{\gamma}_t\cdot\boldsymbol{p}) = -\omega_B(\boldsymbol{p} \wedge \hat{\boldsymbol{B}})\cdot\nabla_p(\boldsymbol{\gamma}_t\cdot\boldsymbol{p}) . \tag{A.5}$$

In section 3 we encountered operators that are functions of the combination $z - L_0^B$, with $\mathrm{Im}\, z > 0$. In particular, we needed an explicit expression for the result of the action of such an operator $F(z - L_0^B)$ on an arbitrary function $f(\boldsymbol{p}, z)$. For convenience we limit ourselves to functions $F(z)$ that are analytic in z in the upper half-plane. To evaluate such an expression we start by rewriting it as follows:

$$F[z - L_0^B(\boldsymbol{k},\boldsymbol{p})] f(\boldsymbol{p}, z) = -\mathrm{i}\int_0^\infty \mathrm{d}t\; \mathrm{e}^{\mathrm{i}zt} F(t)\, \mathrm{e}^{-\mathrm{i}L_0^B(\boldsymbol{k},\boldsymbol{p})t} f(\boldsymbol{p}, z) , \tag{A.6}$$

with $F(t)$ the inverse Laplace transform of $F(z)$,

$$F(t) = \frac{\mathrm{i}}{2\pi}\int_{-\infty+\mathrm{i}0}^{\infty+\mathrm{i}0} \mathrm{d}z\; \mathrm{e}^{-\mathrm{i}zt} F(z) . \tag{A.7}$$

Employing (A.2) in the right-hand side of (A.6) we get

$$F[z - L_0^B(\boldsymbol{k},\boldsymbol{p})] f(\boldsymbol{p}, z) = -\mathrm{i}\int_0^\infty \mathrm{d}t\; \mathrm{e}^{\mathrm{i}zt} F(t)\, \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{\alpha}_t\cdot\boldsymbol{p}/m} f(\boldsymbol{\gamma}_t\cdot\boldsymbol{p}, z) , \tag{A.8}$$

or, with the use of the convolution theorem for Laplace transforms

$$F[z - L_0^B(\boldsymbol{k},\boldsymbol{p})]f(\boldsymbol{p},z) = -\int_0^\infty \mathrm{d}t\,\mathrm{e}^{\mathrm{i}zt}\int_0^t \mathrm{d}\tau\,F(\tau)\,\mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{\alpha}_\tau\cdot\boldsymbol{p}/m}f(\gamma_\tau\cdot\boldsymbol{p},t-\tau)\,, \qquad \text{(A.9)}$$

with $f(\boldsymbol{p},t)$ the inverse Laplace transform of $f(\boldsymbol{p},z)$. As a useful example we consider these formulae for the case $F(z)=z^{-1}$, so that $F(t)=1$. Then (A.8) and (A.9) become

$$[z - L_0^B(\boldsymbol{k},\boldsymbol{p})]^{-1}f(\boldsymbol{p},z) = -\mathrm{i}\int_0^\infty \mathrm{d}t\,\mathrm{e}^{\mathrm{i}zt}\,\mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{\alpha}_t\cdot\boldsymbol{p}/m}f(\gamma_t\cdot\boldsymbol{p},z)$$

$$= -\int_0^\infty \mathrm{d}t\,\mathrm{e}^{\mathrm{i}zt}\int_0^t \mathrm{d}\tau\,\mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{\alpha}_\tau\cdot\boldsymbol{p}/m}f(\gamma_\tau\cdot\boldsymbol{p},t-\tau)\,. \qquad \text{(A.10)}$$

Trivial generalizations of the formulae (A.9)–(A.10) have been used in section 3, in (3.5) and (3.16).

Appendix B

Asymptotic expansions for $J_{L'}$

In this appendix the asymptotic expansions for the contribution $J_{L'}(b,\Gamma)$ to the inverse self-diffusion coefficient (4.9) are presented. To derive these expansions use will be made of the representation (4.10).

In paper II we have derived the asymptotic expansions for the function $K(x)$

$$K(x) \simeq \frac{1}{2x}(1-3x^2) \qquad (x \ll 1)\,, \qquad \text{(B.1a)}$$

$$K(x) \simeq \frac{1}{40x^3}\left[1+\frac{15\zeta(3)}{2\pi^{5/2}x}+\frac{1}{8x^2}\right] \qquad (x \gg 1)\,. \qquad \text{(B.1b)}$$

To derive the asymptotic expansion of $J_{L'}(b,\Gamma)$ for $b \ll 1$ we split the integration interval in (4.10) into $[0,x_0]$ and $[x_0,X/b]$, with x_0 chosen such that $x_0 \gg 1$ and $bx_0 \ll 1$. For $x \le x_0$ we use $x^2/(b^{-2}+x^2) \simeq b^2x^2$. On the other hand, if $x \ge x_0$ we replace $K(x)$ by its asymptotic expansion (B.1b). As a consequence we obtain

$$J_{L'}(b,\Gamma) \simeq -\frac{1}{40}b^2\log b + C_1b^2 - \frac{3\zeta(3)}{32\pi^{3/2}}b^3 + \mathcal{O}(b^{4-\delta})\,, \qquad \text{(B.2)}$$

for arbitrarily small $\delta > 0$. The constant C_1 is given by

$$C_1 = \int_0^{x_0} \mathrm{d}x\, x^2 K(x) - \frac{1}{40}\log x_0 . \tag{B.3}$$

For $x_0 \gg 1$ it is independent of x_0; numerically we have found $C_1 = 0.0972$.

For $b \gg 1$ we must distinguish two cases. If $X/b \ll 1$ we may use (B.1a) in (4.10). Then the leading contribution of

$$J_{L'}(b, \Gamma) \simeq \tfrac{1}{2} \int_0^{X/b} \mathrm{d}x \frac{x}{b^{-2} + x^2}(1 - 3x^2) \simeq \tfrac{1}{4}\log(1 + X^2) \simeq -\tfrac{1}{2}\log(\sqrt{3}\Gamma^{3/2}) \tag{B.4}$$

for $b \to \infty$ and $\Gamma \ll 1$. Insertion into (4.9) immediately yields (4.12) again. If, on the other hand, $b \gg 1$, but not $X/b \ll 1$, we choose $x_0 \ll 1$ such that $bx_0 \gg 1$ and split the integration in (4.10) at x_0. Then we may use $x^2/(b^{-2} + x^2) \simeq 1 - b^{-2}x^{-2}$ if $x \geq x_0$; for $x \leq x_0$ we replace $K(x)$ by its asymptotic expression (B.1a). In this way we get

$$J_{L'}(b, \Gamma) \simeq \tfrac{1}{2}\log b + C_2 + \mathcal{O}(b^{-2+\delta}) \tag{B.5}$$

for arbitrarily small $\delta > 0$. The constant C_2 is defined as

$$C_2 = \int_{x_0}^{X/b} \mathrm{d}x\, K(x) + \tfrac{1}{2}\log x_0 . \tag{B.6}$$

For $x_0 \ll 1$ and $X/b \gg 1$ it is independent of both x_0 and X/b. Numerically we have found $C_2 = -0.406$.

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