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Dynamics of classical plasmas

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The recent theory of Raedt and Raedt (RR) is analyzed and applied to study the dynamics of a classical one-component plasma. It is shown that this method is very similar to making the Lovesey approximation (for the calculation of the memory function involved) at an appropriate stage of the continued fraction hierarchy for the memory function. The expression for the density-fluctuation spectrum obtained by using RR theory is then evaluated for the entire density range for which molecular dynamics data are available. For smaller q values the results obtained are of similar quality to those obtained recently by this author using a renormalized free-particle memory function, and compare well with the data. However, for larger q values a shoulder appears at high frequencies which is not observed in the molecular-dynamics results.

I. INTRODUCTION

Recently there has been considerable interest[1-8] in the study of dynamical correlations in a classical one-component plasma (OCP) which essentially consists of an assembly of identical point charges moving classically in a uniform neutralizing background which is assumed to be inert. This system, which serves as a reference system for charged fluids, is of direct interest in the study of astrophysical plasmas where the motion of the ions can be treated classically and the background is provided by the degenerate electrons. The thermodynamic state of the system is described by the coupling parameter $\Gamma = (Ze)^2/r_0 k_B T$, where r_0 is the radius of a sphere containing one single ion at the given ion density and the other symbols have their usual meaning; Γ is effectively the ratio of potential energy to the kinetic energy and thus characterizes the system.

The stimulus for studying the dynamics of OCP was provided by the molecular-dynamics (MD) data of Hansen *et al.*[1] for the longitudinal and transverse correlations. The main theoretical attempts have been extensions of the kinetic theory[3,4] and the mode-coupling theory[5] of classical liquids. The latter theory gives a better description of the MD data, especially with a Lorentzian form for the relaxation kernel. These calculations are very involved computationally and are done only for selected values of Γ. For example, the calculation[4] using kinetic theory could not be carried over for larger values of Γ, since no self-consistency is achieved within a reasonable computational time.

In a recent paper[6] (hereafter referred to as I) the behavior of the dynamical structure factor $S(q,\omega)$ has been studied, using its frequency-moment sum rules. These sum rules are the exact coefficients in the high-frequency expansion of the correlation functions and can be calculated from a knowledge of static correlation functions and the interparticle potential only. In I, the result is given for the sixth-moment sum rule[7] of $S(q,\omega)$, which can be computed easily for any general wave vector. In order to calculate $S(q,\omega)$, the third-order memory function in the continued-fraction expansion[9] of the Laplace transform of the density correlation function is approximated by a renormalized[10,11] free-particle memory function (MF). The renormalization parameter is determined by using the sixth frequency moment. The results obtained for the dynamical structure factor are in reasonably good agreement with the MD data. $S(q,\omega)$ of classical OPC has also been studied[8] by including the backflow effects through the effective-mass parameter in mean-field theory. This parameter is determined using results[6] for the sixth-moment sum rule. The results obtained for $S(q,\omega)$ are quite reasonable for the values of q and Γ shown there.

The purpose of the present paper is to analyze the recent theory of Raedt and Raedt[12,13] (RR) and to apply it to the system of a classical one-component plasma. RR have successfully employed their method to study the dynamics of the Heisenberg chain[12] and of an electron liquid.[13] However, they have grossly approximated the fifth frequency moment of $S(q,\omega)$, which is not known for an electron liquid. Furthermore, in all the moments the terms involving the static structure factor $S(q)$ were replaced by some adjustable parameters which they chose after some consideration.[13] The quality of their results is better than that of earlier ones.[11,14] However, it remains to be seen how good these results are when instead actual information is fed into the theory. It is with this intention that I thought it worthwhile to apply

this method to a classical OCP, where we are better off because the higher (sixth) frequency moment of $S(q,\omega)$ is known[6] exactly and $S(q)$ is also available from a Monte Carlo calculation.[15] In doing so I also show that if the MF at the fourth stage of the continued fraction is approximated by its $\omega=0$ value, then the expression obtained for the third-order memory function is almost identical to the one obtained by following RR theory and that they hardly differ numerically, especially for small wave vectors. I then calculate the dynamical structure factor for the entire range of plasma parameters Γ, and the results are compared with those obtained in I and also with the MD data.

The paper is organized as follows. In Sec. II, I start with basic definitions and give a few essentials of the RR method as applied to classical OCP. In the last part of Sec. II, the similarity between results obtained using the RR method and those with the Lovesey approximation (at an appropriate stage) is shown. The numerical results are given and discussed in Sec. III. Section IV contains some concluding remarks.

II. GENERALITIES

A. Basic definitions

The dynamics of longitudinal correlations can be conveniently described in terms of a density-density correlation function

$$S(\vec{q},t)=(1/N)\langle\rho^{\dagger}(\vec{q},t)\rho(\vec{q},0)\rangle\,, \tag{2.1}$$

where N is the total number of particles of the species under consideration and the angular brackets denote the thermal average; $\rho(\vec{q},t)$ is the density-fluctuation operator and is defined as

$$\rho(\vec{q},t)=\sum_{j=1}^{N}\exp[-i\vec{q}\cdot\vec{r}_j(t)]\,, \tag{2.2}$$

where $\vec{r}_j(t)$ is the position coordinate of the jth particle at time t. We are interested in the study of the dynamical structure factor $S(q,\omega)$, which is the Fourier transform of $S(q,t)$; i.e.,

$$S(q,\omega)=\frac{1}{2\pi}\int_{-\infty}^{\infty}dt\,e^{i\omega t}S(q,t)\,. \tag{2.3}$$

Owing to rotational invariance of the system, $S(q,\omega)$ and the other averaged quantities depend only on the magnitude of the wave vector $\vec{q}$.

In the memory-function formalism[9] it is convenient to work with the Laplace transform of the density correlation function, which is defined as

$$S(q,z)=\int_{0}^{\infty}dt\,e^{izt}S(q,t)\,, \tag{2.4}$$

where $z=\omega+i\epsilon$, ϵ being a positive infinitesimal. It follows from (2.3) and (2.4) that

$$S(q,\omega)=(1/\pi)\,\mathrm{Re}S(q,z)\,. \tag{2.5}$$

In order to make a connection with the method and notation[16] of RR, it can be seen by integrating (2.4) that

$$S(q,z)=(i/N\beta)\phi_{\rho,\rho}(q,z)\,, \tag{2.6}$$

where $\phi_{\rho,\rho}(q,z)$ is the Laplace transform of the density-density relaxation function[13] and is given by

$$\phi_{\rho,\rho}(q,z)=\left(\rho(q),\frac{1}{z-L}\rho(q)\right). \tag{2.7}$$

Here L is the classical Liouville operator which generates the time evolution of any operator according to $G(t)=e^{iLt}G(0)$. In Eq. (2.7) and all following equations, the scalar product of any two operators is defined as

$$(G,F)=\beta\langle G^{\dagger}F\rangle\,. \tag{2.8}$$

It is because of this relatively simple definition of the scalar product (as compared to that for a quantum plasma) that the simple relationship (2.6) exists between the correlation function and the relaxation function of the same dynamical variable.

Before going to the actual MF formalism, I give the expressions for the various frequency-moment sum rules which appear in this method in a natural way. For $S(q,\omega)$ these sum rules are defined as

$$\langle\omega^{2n}(q)\rangle=\int_{-\infty}^{\infty}d\omega\,\omega^{2n}S(q,\omega)\,. \tag{2.9}$$

Hereafter q and r are measured in units of r_0^{-1} and r_0, respectively, and various moments are expressed in the appropriate powers of the classical plasma frequency of the ions. The results for the low-order[6,7] moments are

$$\langle\omega^2(q)\rangle=\omega_0^2(q)=q^2/3\Gamma\,, \tag{2.10}$$

$$\langle\omega^4(q)\rangle=\omega_0^2[1+3\omega_0^2+2I(q)]\,, \tag{2.11}$$

$$\begin{aligned}\langle\omega^6(q)\rangle=\omega_0^2(15\omega_0^2+\tfrac{37}{5})+36\omega_0^2\int_0^{\infty}\frac{dr}{r}\,[g(r)-1]\,\frac{j_3}{qr}\\ +\tfrac{4}{3}\int_0^{\infty}\frac{dr}{r^4}\,g(r)(1-j_0+j_2)\\ +[1+2I(q)]^2+I_3(q)\,.\end{aligned} \tag{2.12}$$

In these equations the argument of the Bessel functions is understood to be qr, and

$$I(q)=\int_0^{\infty}\frac{dr}{r}[g(r)-1]j_2\,. \tag{2.13}$$

Further, $I_3(q)$ is the explicit three-body contribution to the sixth frequency moment of $S(q,\omega)$ and is given by[6]

$$I_3(q)=\frac{1}{2}\iint_0^\infty \frac{dr}{r}\frac{dr'}{r'}\left(1-4j_0+\frac{6}{qr}j_1\right)\int_{-1}^{1}d\gamma(3\gamma^2-1)[g_3(r,r',\gamma)-g(r)g(r')]$$
$$+\frac{1}{2}\iint_0^\infty dr\,dr'\int_{-1}^{1}d\gamma[g_3(r,r',\gamma)-g(R)g(r')]$$
$$\times\frac{1}{R^3}\left(\frac{r^2}{r'}\left(j_0-\frac{3}{qr}j_1\right)(1-3\gamma^2)-\frac{3r^2}{R^2}\left\{\frac{r^2}{r'}\left(j_0-\frac{2}{qr}j_1\right)-\frac{2r'}{qr}j_1+r\left(j_0+\frac{j_1}{qr}\right)\gamma\right.\right.$$
$$\left.\left.-\left[2r'\left(j_0-\frac{3}{qr}j_1\right)+\frac{3r^2}{r'}\left(j_0-\frac{2}{qr}j_1\right)\right]\gamma^2+3r\left(j_0-\frac{3}{qr}j_1\right)\gamma^3\right\}\right). \tag{2.14}$$

Here $R=|\vec{r}-\vec{r}'|$; $g(r)$ and $g_3(r,r',\gamma)$ are respectively the static two- and three-particle distributions functions of the system. In what follows we shall use these results frequently.

B. Three-variable theory of RR

I briefly give here the essentials of the method of RR as applied to classical OCP. For details, the reader is referred to their papers.[12,13] This method consists of using a set of slow variables as the relevant variable in the generalized Langevin equation and then determining the MF involved from its equation of motion in z space, using a sum rule. Total density being a conserved quantity, I also chose[13] the set of slow variables as

$$E(\vec{q})=\{\rho(\vec{q}),L\rho(\vec{q}),A(\vec{q})\}. \tag{2.15}$$

where

$$A(\vec{q})=L^2\rho(\vec{q})-(L\rho(\vec{q}),L\rho(\vec{q}))/(\rho(\vec{q}),\rho(\vec{q}))\rho(\vec{q}). \tag{2.16}$$

This particular form of $A(q)$ ensures orthogonality among different elements of the set (2.15). For simplicity of notation, hereafter the arguments of E, ρ, A and various frequency moments are suppressed.

The Laplace transform of the generalized Langevin equation for the E-E relaxation function is given by[9]

$$[z\tilde{1}-\tilde{\Omega}(q)+i\tilde{M}(q,z)]\cdot\tilde{\phi}(q,z)=N\beta\tilde{S}(q), \tag{2.17}$$

where $\tilde{S}(q)=(E,E)/N\beta$ and $\tilde{1}$ denotes a unit matrix. Further,

$$\tilde{\Omega}(q)=(E,LE)\cdot(E,E)^{-1} \tag{2.18}$$

is the frequency matrix, where the dot indicates matrix multiplication. The matrix of relaxation functions is given by

$$\tilde{\phi}(q,z)=(E,(z-L)^{-1}E), \tag{2.19}$$

and the memory matrix $\tilde{M}(q,z)$ is the Laplace transform of

$$\tilde{M}(q,t)=(f(t),f)\cdot(E,E)^{-1}. \tag{2.20}$$

Here

$$f(t)=e^{t(1-P)iL}(1-P)iLE \tag{2.21}$$

is the random force vector associated with the variable E. In Eq. (2.21) P is a projection operator which projects any operator G on the three-dimensional subspace E, according to[13]

$$PG=\frac{(\rho,G)}{(\rho,\rho)}\rho+\frac{(L\rho,G)}{(L\rho,L\rho)}L\rho+\frac{(A,G)}{(A,A)}A. \tag{2.22}$$

The expressions for the matrices $\tilde{S}(q)$, $\tilde{\Omega}(q)$, and $\tilde{M}(q,z)$ are simplified by means of the time-reversal invariance of the correlation functions involved and further by using the fact that the different vectors of the subspace E are orthogonal. The results obtained for classical OCP are given by

$$\tilde{S}(q)=S(q)\begin{pmatrix}1&0&0\\0&\delta_1^2&0\\0&0&\delta_1^2\delta_2^2\end{pmatrix}, \tag{2.23}$$

$$\tilde{\Omega}(q)=\begin{pmatrix}0&1&0\\\delta_1^2&0&1\\0&\delta_2^2&0\end{pmatrix}, \tag{2.24}$$

$$\tilde{M}(q,z)=\begin{pmatrix}0&0&0\\0&0&0\\0&0&-i\Sigma(q,z)\end{pmatrix}, \tag{2.25}$$

where

$$\delta_1^2=\frac{\langle\omega^2\rangle}{S(q)},\quad \delta_2^2=\frac{\langle\omega^4\rangle}{\langle\omega^2\rangle}-\frac{\langle\omega^2\rangle}{S(q)}. \tag{2.26}$$

Further,

$$\Sigma(q,z)=\frac{-1}{(A,A)}\left(QLA,\frac{1}{z-QLQ}QLA\right), \tag{2.27}$$

where $Q=1-P$. Employing Eqs. (2.23)–(2.25) in Eq. (2.17), one obtains an expression for $\phi_{\rho,\rho}(q,z)$ by solving three equations simultaneously. Using this expression in Eq. (2.6), we obtain the following expression for the Laplace transform of the density correlation function:

$$S(q,z)=\frac{S(q)[z^2+z\Sigma(q,z)-\delta_2^2]}{iz(\omega_l^2-z^2)+i\Sigma(q,z)(\delta_1^2-z^2)}, \qquad (2.28)$$

where $\omega_l^2=\langle\omega^4\rangle/\langle\omega^2\rangle$. We now proceed to determine $\Sigma(q,z)$, following the prescription of RR.

The identity

$$z(z-QLQ)^{-1}=1+QLQ(z-QLQ)^{-1},$$

when applied twice on Eq. (2.27), yields the following equation of motion for the MF:

$$(z^2+\delta_2^2+\delta_3^2)\Sigma(q,z)$$

$$=-z\delta_3^2-(A,A)^{-1}\left(QL^3A,\frac{1}{z-QLQ}QLA\right), \qquad (2.29)$$

where

$$\delta_3^2=\left[\frac{\langle\omega^6\rangle}{\langle\omega^2\rangle}-\left(\frac{\langle\omega^4\rangle}{\langle\omega^2\rangle}\right)^2\right]\Big/\delta_2^2. \qquad (2.30)$$

The last term on the right-hand side of Eq. (2.29) involves higher-order derivatives and is replaced[12,13] by a frequency-independent constant R. Taking the limit $z=i\epsilon$, $\epsilon\to 0$ in Eq. (2.29) yields

$$(\delta_2^2+\delta_3^2)\lim_{\epsilon\to 0}\Sigma(q,i\epsilon)=-R. \qquad (2.31)$$

From symmetry[12] it can be seen that the real part of $\lim_{\epsilon\to 0}\Sigma(q,i\epsilon)$ is zero, so that R is purely imaginary. It is calculated by means of Eq. (2.29) and the following sum rule[13] for the memory function:

$$\frac{(QLA,QLA)}{(A,A)}$$

$$=\frac{1}{2\pi i}\lim_{\epsilon\to 0}\int_{-\infty}^{\infty}d\omega[\Sigma(q,\omega+i\epsilon)-\Sigma(q,\omega-i\epsilon)]. \qquad (2.32)$$

The result obtained is

$$R=-i\delta_3^2\tau_R^{-1},\quad \tau_R^{-1}=(\delta_2^2+\delta_3^2)^{1/2}. \qquad (2.33)$$

Using (2.33) in Eq. (2.29) leads to the following expression for the MF:

$$\Sigma(q,z)=-\delta_3^2/(z+i\tau_R^{-1}). \qquad (2.34)$$

Thus τ_R is a relaxation time determining the decay of the memory function. Further, the quantities δ_1^2, δ_2^2, and δ_3^2 are the $t=0$ values of the first-, second-, and third-order memory functions in the continued-fraction expansion obtained using the density-fluctuation operator as the only variable.

C. Connection with earlier work

As the set of different variables in the multivariable theory of RR is constituted by the main variable and its subsequent derivatives, their method is formally equivalent to a single-variable method[6,9-11,17] in which one goes lower in the continued-fraction hierarchy:

$$S(q,z)=S(q,t=0)/[-iz+M_n(q,z)], \qquad (2.35)$$

$$M_n(q,z)=M_n(q,t=0)/[-iz+M_{n+1}(q,z)]. \qquad (2.36)$$

Here $M_n(q,z)$ is the Laplace transform of the MF entering at the nth stage of the expansion, when only one variable, $\rho(q)$, is used in the Langevin equation. In fact, even for quantum electron liquid, it can be seen that the expression for the relaxation function as obtained by RR[13] using three variables is exactly the same as that derived earlier by myself and co-workers.[11] Thus their remark[13] that only two variables were used in the calculation in Ref. 11 is incorrect. In fact, in that calculation[11] we used the density-fluctuation operator as the only variable and carried out the MF expansion up to the third[18] stage.

Similarly the expression for $S(q,z)$ employed in I is identical to that given by Eq. (2.28), since the exact expressions for $M_3(q,z)$ and $\Sigma(q,z)$ are related by

$$M_3(q,z)=-i\Sigma(q,z). \qquad (2.37)$$

However, as we see in Sec. III, they lead to quite different results for the density-fluctuation spectra, since the approximation for the memory function is entirely different in the two cases. Prior to that, we show that if the fourth-order MF is assumed to be a constant, the resulting expression for $M_3(q,z)$ is identical to the one obtained in the RR approximation.

From Eq. (2.36) one can write

$$M_3(q,z)=M_3(q,t=0)/[-iz+M_4(q,z)]. \qquad (2.38)$$

Assuming that $M_4(q,z)$ decays faster than $M_3(q,z)$, we approximate $M_4(q,z)$, following Lovesey,[17] by a decay constant whose value is given by the $z=0$ value of the MF; i.e.,

$$M_4(q,z)=\tau_P^{-1}(q)=M_4(q,z=0). \qquad (2.39)$$

τ_P^{-1} can be estimated by relating $M_4(q,z=0)$ to $M_2(q,z=0)$ through Eq. (2.36) and further assuming[17] $M_2(q,t)$ to be a function of $M_3(q,t=0)t^2$, which amounts to incorporating correctly the short-time behavior of the MF. We consequently obtain

$$\tau_P^{-1}=\xi\delta_3, \qquad (2.40)$$

and thus expression (2.38) in this approximation

becomes

$$M_3(q, z) = \delta_3^2/(-iz + \tau_P^{-1}). \tag{2.41}$$

The constant ξ in Eq. (2.40) can be fixed through any physical property of the system.[17,19] We determine it by demanding that $S(q, z=0)$ [obtained by substituting (2.41) in Eq. (2.35)] correctly reproduces its free-particle limit. This yields $\xi = (\frac{3}{8\pi})^{1/2}$.

The similarity between the memory functions given by Eqs. (2.34) and (2.41) is worth noticing. They differ only in relaxation times. In Sec. III we see that there is only a little difference between the numerical values of τ_R^{-1} and τ_P^{-1}, so that the quality of the results obtained using these two approximations is exactly the same.

III. NUMERICAL RESULTS AND DISCUSSION

We now evaluate numerically the dynamical structure factor, the expression for which can be written from Eqs. (2.5) and (2.28) as

$$S(q, \omega) = \frac{S(q)}{\pi} \frac{\delta_1^2 M'(q, \omega)}{[(\omega^2 - \delta_1^2) - \omega M''(q, \omega)]^2 + [\omega M'(q, \omega)]^2}. \tag{3.1}$$

This is intentionally written in terms of a lower-order MF, $M(q, z)$, since we shall be discussing the results in terms of this MF. Its real (M') and imaginary (M'') parts can be calculated from

$$M(q, z) = i\delta_2^2/[z + \Sigma(q, z)] \equiv \delta_2^2/[-iz + M_3(q, z)]. \tag{3.2}$$

The calculation of $S(q, \omega)$ obviously requires the knowledge of its frequency moments up to the sixth, which are calculated from the exact expressions (2.10)–(2.12). The data for $g(r)$ required in the calculation of $\langle\omega^4\rangle$ and $\langle\omega^6\rangle$ are taken from the Monte Carlo study[15,20] of this correlation function. Since no comparable information is available about the triplet correlation function, the last term in $\langle\omega^6\rangle$ is evaluated by using[6] the superposition approximation for $g_3(r, r', \gamma)$. This approximation is quite good for the calculation of frequency moments in classical liquids, as is shown by the recent[21] molecular-dynamics calculation, and there seems to be no reason to expect the opposite in the present case. For the remaining static quantity $S(q)$, the Monte Carlo numbers obtained by Hansen[15] are used.

The calculation of $S(q, \omega)$ is carried out for the entire range of the plasma parameter Γ and the wave vector $\vec{q}$, using different approximate forms for the MF in Eq. (3.2) as given by Eqs. (2.34) and (2.41). The results obtained are presented in Figs. 1–3 for three different values of Γ. They are compared with the molecular-dynamics data[1] and the corresponding results obtained[6] using the renormalized free-particle form of $M_3(q, z)$. For all Γ, results of $S(q, \omega)$ obtained using the MF (2.41) are of the same quality as those obtained from the MF (2.34) and are therefore shown only for $\Gamma = 9.7$. This is because these two memory functions differ only in their relaxation times τ_R and τ_P, whose values are very close to each other, especially at small wave vectors. Thus these two results hardly can be distinguished for all Γ for small values of q. As q increases, the values of τ_R and τ_P begin to deviate from each other, but the quality of the two results remains essentially the same (see Fig. 1). Therefore we

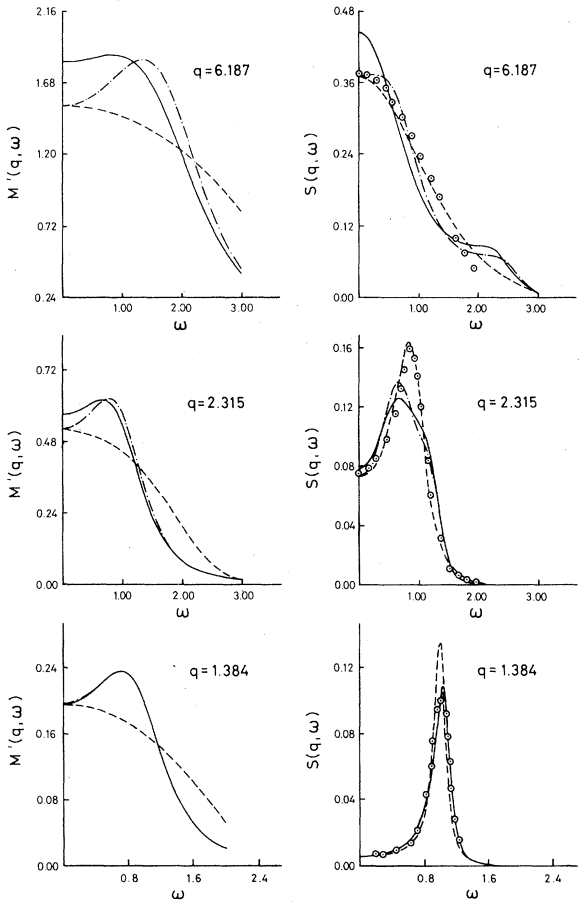

FIG. 1. Real part $M'(q, \omega)$ of the memory function (3.2) and the corresponding dynamical structure factor $S(q, \omega)$ for $\Gamma = 9.7$. Results are shown as a function of ω for $q = 1.384$, 2.315, and 6.187. Solid curves show the present results obtained using the RR method [MF (2.34)]. Dot-dashed curve represents results obtained using Lovesey approximation [MF (2.41)] at one stage higher than usual. Dashed curve represents results obtained by using the renormalized free-particle MF (Ref. 6). Centered circles are MD results for $S(q, \omega)$ taken from Ref. 1.

are concerned only with the results obtained using the RR approximation, i.e., those obtained using the MF (2.34).

For the smallest q for which MD data are available, the plasmon peak in the present calculation is sharper as in I also and is shown only for $\Gamma = 110.4$. For other values of Γ, the quality of the results is similar. For the next-higher values of q (i.e., $q = 1.384$ for $\Gamma = 9.7$ and $q = 1.856$ for $\Gamma = 110.4$ and 152.4), the present results are a little better. But for the remaining large values of q, the renormalized MF gives a better representation of the MD data. This is because for large q the renormalized MF leads to exact free-particle behavior of $S(q, \omega)$, which does not occur in the present case.

The characteristic feature of the present results is the two-peak structure of $S(q, \omega)$, one of which appears as the main peak and the other as a shoulder which is clearly visible for large wave vectors. The main peak is reminiscent of the collective plasma oscillations and occurs at a frequency where the denominator on the right-hand side of Eq. (3.1) is minimum. The origin of the shoulder can be traced back to the maxima in the real part $M'(q, \omega)$ of the memory function (3.2). It can be seen that $M'(q, \omega)$ can always exhibit a maxima on the positive ω side if the condition

$$2\delta_3^2 > \tau^{-2} \tag{3.3}$$

is satisified (where τ can be τ_R or τ_P). By using the actual values of the frequency moments we find that this condition is always satisified when τ is given by either (2.33) or (2.40). Therefore $M'(q, \omega)$ exhibits a maxima on the positive side for all values of q and ω. The position of the peak when $\tau = \tau_R$ is seen to be given by

$$\omega_{\max}^2 = \tfrac{1}{2}(\delta_3^2 - \delta_2^2) . \tag{3.4}$$

For $\Gamma = 9.7$ the results for $M'(q, \omega)$ are shown in Fig. 1 and are compared with the corresponding results obtained using the renormalized free-particle approximation, which do not show any such maxima, exhibiting instead maxima at $\omega = 0$. The behavior of $M'(q, \omega)$, as depicted in Fig. 1, is typical of other values of Γ also. It may be noted that the maximum at $\omega \simeq 0.7$ in $M'(q, \omega)$ for $q = 1.384$ does not show up in the corresponding results for $S(q, \omega)$. It is suppressed because of the comparatively large magnitude of the denominator in Eq. (3.1) for this frequency range. However, as q increases, this peak gives rise to an apparent shoulder in the curves for $S(q, \omega)$, as can be seen in Figs. 1–3. For example, when $\Gamma = 9.7$, the results[22] obtained using renormalized MF show only one peak for $q = 2.315$ and 6.187 and are in agreement with the MD results, but the present results using the RR method show a high-frequency shoulder.[23] For $\Gamma = 110.4$ the behavior of $S(q, \omega)$ for $q = 6.187$ (not shown in Fig. 2) is of the same type as the corresponding results for $\Gamma = 152.4$ (shown in Fig. 3) and does show a shoulder around $\omega \simeq 0.9$. The only indication of a shoulder in the MD results is for $q = 3.094$ for $\Gamma = 110.4$ and 152.4. In the present calculation these shoulders are stronger and occur at slightly lower frequencies, compared to the MD data. I have not given here the results for $\Gamma = 0.993$, since they also show similar behavior: for small q agreement is reasonable with the MD results, but again a high-frequency shoulder appears for large values of q.

I have ascertained that the shoulder in $S(q, \omega)$ is not a consequence of some error due to the use of the superposition approximation in the numerical evaluation of $\langle \omega^6 \rangle$. This is because the explicit three-body contribution $I_3(q)$ (it is only this term which is evaluated using the superposition approximation) to the total moment is very small.[24] The most dominant contribution for large wave vectors comes from kinetic terms. For example, for $q = 6.187$, $I_3(q)$ is even less than 1% of $\langle \omega^6 \rangle$ for $\Gamma \leq 10$ and increases to about 10% of $\langle \omega^6 \rangle$ for $\Gamma = 152.4$. Therefore a larger error in $I_3(q)$

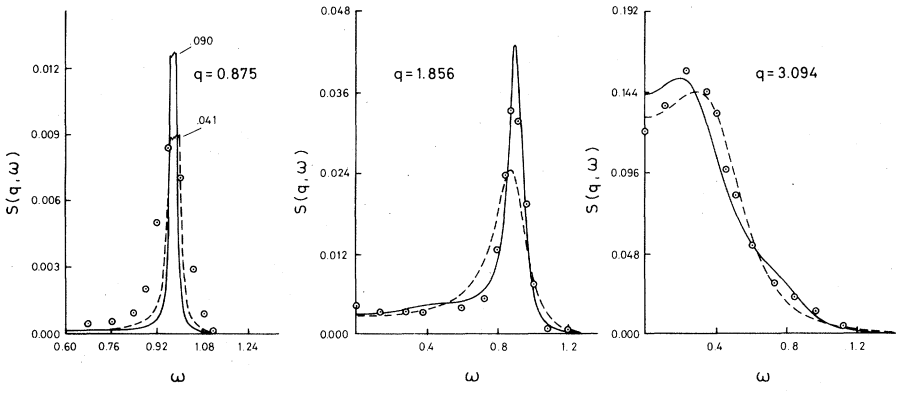

FIG. 2. Dynamical structure factor $S(q, \omega)$ as a function of ω for indicated values of q for $\Gamma = 110.4$. Curves have same meaning as in Fig. 1.

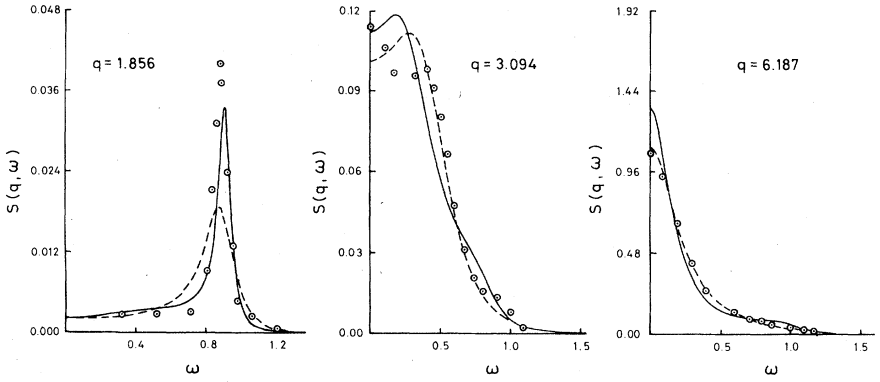

FIG. 3. Same as Fig. 2, but for $\Gamma = 152.4$.

would lead to a very small error in $\langle\omega^6\rangle$. We have seen that changing $I_3(q)$ by as much as 30% of its value (calculated using the superposition approximation) leaves the quality of results for $S(q,\omega)$ unchanged.

IV. CONCLUDING REMARKS

I have analyzed and applied the theory of Raedt and Raedt for studying the dynamical structure factor of a classical one-component plasma. The calculation is carried over a wide range of densities and wave vectors, and the results are compared with those obtained in I and with the molecular-dynamics data. For small q they are in reasonably good agreement with the MD data. But this agreement is lost for large wave vectors, owing to the appearance of a side shoulder in the spectrum. We note that this shoulder emerges as a consequence of the peak in the MF (3.2) at a nonzero frequency. On the other hand, there is no such peak when this MF is evaluated by means of a renormalized free-particle approximation,[6] which consequently gives a better description of the data over the entire range of q and Γ. This is in contrast to what is found in studying $S(q,\omega)$ of electrons in metals for which the RR method seems to work better.[13] This might be due to the fact that an experimental $S(q,\omega)$ of electrons in metals does exhibit a two-peak structure which is built into the RR approximation, whereas in the case of classical OCP the density-fluctuation spectrum essentially contains a single peak.

It is also shown that the RR prescription of calculating the MF is similar in spirit to making a Lovesey-type[17] approximation at one stage higher than usual, in the continued-fraction expansion for the correlation function. That is why the results obtained using the latter approximation are essentially of the same quality as those obtained using the RR method and are shown only for $\Gamma = 9.7$. However, the arguments given by RR are more convincing once the last term on the right-hand side of the equation of motion (2.29) is assumed to be constant. It may be further noted that all three approximations discussed satisfy the same number (i.e., up to the sixth) of frequency-moment sum rules of $S(q,\omega)$ and do not involve any adjustable parameter.

We have confined ourselves to the study of longitudinal correlations. For studying transverse-current correlations I feel that the RR method (or the Lovesey-type approximation for the fourth-order MF in the continued-fraction hierarchy) should be quite suitable. This is because the transverse-current spectrum $C_t(q,\omega)$ exhibits[1] a two-peak structure for large q which is in principle built into this approximation using three variables. However, for that one would require the knowledge of the sixth frequency moment of $C_t(q,\omega)$, which involves complicated four-body correlations. Still, it might be worthwhile to keep this moment as a parameter and fix it through the best fit of the results for $C_t(q,\omega)$ with the molecular-dynamics data.

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[24]See Table I of Ref. 6.