Dynamic structure factor of a two-dimensional electron gas

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The dynamic structure factor $S(k,\omega)$ of a two-dimensional electron gas is calculated at $r_s=1$ and 5 within the Mori memory function formalism. We use the Gaussian model for the memory function at second stage and obtain the necessary static inputs from the quantum Monte Carlo calculation by Tanatar and Ceperley and Moroni, Ceperley, and Senatore. $S(k,\omega)$ thus calculated shows a clear two-peak structure in the intermediate wave-vector domain beyond the plasmon cutoff wave vector at both $r_s=1$ and 5. The results are compared with the quantum Singwi-Tosi-Land-Sjölander (QSTLS) theory and the calculation of Tanatar. It is found that our results are similar to that of QSTLS at $r_s=5$ and do not support the Tanatar prediction of finding only a single broad peak at intermediate k. [S0163-1829(96)07035-X]

I. INTRODUCTION

The dynamic structure factor $S(k,\omega)$ is a fundamental quantity in describing the excitation spectrum of the interacting many-electron systems and its study in two dimensions has gained a good deal of interest in recent years. This arises mainly from the possibility of its experimental measurement due to the exact physical realization of two-dimensional (2D) electron systems in the laboratory, which include the electrons at the interfaces of semiconductor hetrojections; for example, the silicon metal-oxide-semiconductor and the $GaAs/Al_xGa_{1-x}As$ superlattice structure. The electrons trapped on the liquid helium surface constitute another interesting example of a 2D electron system. However, unlike the 3D case,[1] to the best of our knowledge $S(k,\omega)$ in 2D has not yet been experimentally determined, (for an introduction to the various developments in 2D electron systems see review articles by Ando, Fowler, and Stern[2] and Isihara[3]). Therefore, it becomes both interesting and important to carry out the theoretical study of $S(k,\omega)$ in 2D. In the literature, the electron gas confined to a plane interacting with a $1/r$ potential in the presence of a uniform positive background has been the most widely used model to study the 2D electron systems. A large amount of work has been done on the said 2D electron gas (2DEG) model to understand the various static and dynamic properties of these systems. However, there have been very few attempts to study $S(k,\omega)$ of a 2DEG. In 3D, both experiments[1] and theory[4] predict the two-peak structure in $S(k,\omega)$ at intermediate k beyond the plasmon cutoff wave vector (k_c). Thus, it is quite natural to investigate the possibility of finding the similar two-peak structure in two dimensions also. Lee and Hong[5] have calculated $S(k,\omega)$ for a 2DEG by solving the generalized Langevin equation. However, the applicability of their method is limited to the long-wavelength limit only. Yoshida and Yasuhara[6] used an approximate scheme that took into account the short-range electron correlation effects and the coupling between single-pair and multiple-pair excitations and found that $S(k,\omega)$ thus obtained exhibits a clear double-peak structure in the intermediate wave-vector domain beyond the plasmon cutoff wave vector. The similar behavior of $S(k,\omega)$ has recently been predicted by two of the present authors[7] on the basis of quantum Singwi-Tosi-Land-Sjölander (QSTLS) theory. However, it has been predicted by Tanatar[8] by using the Mori memory function (MF) approach[9] that $S(k,\omega)$ has only a single broad peak at intermediate k. In the Mori formalism the central quantity to calculate is the MF. In the literature there exist different variants of the Mori approach that differ in the method of calculation of the MF. Jindal *et al.*[10] first employed the MF method to calculate $S(k,\omega)$ of a 3DEG. The MF was calculated by renormalizing the free-particle MF and $S(k,\omega)$ thus obtained showed two-peak structure in agreement with the experiments.[1] Yoshida *et al.*[11] introduced the Gaussian model for the MF at second stage and obtained satisfactory results for $S(k,\omega)$ for a 3DEG, but their method involved three adjustable parameters. Tanatar in Ref. 8 extended the model of Yoshida *et al.*[11] to the 2DEG with his calculation involving only one free parameter. All the necessary static inputs, except the isothermal susceptibility $\chi(k)$, were obtained from the quantum Monte Carlo (QMC) calculation.[12] For $\chi(k)$ a lower bound $\chi_{LB}(k)=2S^2(k)/\omega_k[\omega_k=\hbar^2k^2/2m]$ was used and the static structure factor $S(k)$ was taken from the QMC calculation. It was argued that $\chi_{LB}(k)$ is a good approximation for $\chi(k)$, but we now know that it differs considerably from the QMC calculation of Moroni, Ceperley, and Senatore.[13] Therefore, one should expect an improvement in $S(k,\omega)$ results if all necessary static inputs including $\chi(k)$ are taken from the QMC calculation. This in fact forms one of the motivations of doing the present work. Further, we aim to investigate the possibility of observing the double-peak structure in $S(k,\omega)$ of a 2DEG within the MF formalism.

The layout of the paper is organized as follows: The Mori MF formalism is reviewed in brief in Sec. II. The results and

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discussion are given in Sec. III and conclusions are drawn in Sec. IV.

II. MEMORY FUNCTION FORMALISM

In this section we review in brief the Mori MF formalism as used by Yoshida, Takeno, and Yasuhara[11] to study $S(k,\omega)$ of a 3DEG. In this formalism the dynamic density response function $\chi(k,\omega)$ is expressed in terms of a reference response function $\chi^{(0)}(k,\omega)$ and an effective potential $V(k,\omega)$ as

$$\chi(k,\omega)=\frac{\alpha\chi^{(0)}(k,\omega)}{1-V(k,\omega)\chi^{(0)}(k,\omega)}, \tag{1}$$

$$V(k,\omega)=V_0(k)+V_1(k)\omega R_2(k,\omega), \tag{2}$$

where $R_2(k,\omega)=M_2(k,\omega)-M_2^{(0)}(k,\omega)$ is the (normalized) interacting part of the second-order MF such that $R_2(k,t=0)=1$. Here and in what follows the quantity, say X, belonging to the reference system is denoted by $X^{(0)}$. The quantities α, $V_0(k)$, and $V_1(k)$ in the above equations are expressed in terms of frequency moments m_{2p} of the dynamic structure factor $S(k,\omega)$ by

$$\alpha=\frac{m_2}{m_2^{(0)}},\quad V_0=\frac{m_2}{m_2^{(0)}}\left[\frac{1}{m_0}-\frac{1}{m_0^{(0)}}\right],$$

and

$$V_1=\left[\left\{\frac{m_4}{m_2}-\frac{m_4^{(0)}}{m_2^{(0)}}\right\}-\left\{\frac{m_2}{m_0}-\frac{m_2^{(0)}}{m_0^{(0)}}\right\}\right]\Big/\, m_2^{(0)}, \tag{3}$$

with the frequency moments defined as

$$m_{2p}=\int_{-\infty}^{\infty}d\omega\,\omega^{2p-1}S(k,\omega). \tag{4}$$

From the knowledge of $\chi(k,\omega)$, $S(k,\omega)$ is calculated as

$$S(k,\omega)=\frac{\hbar}{\pi}\chi''(k,\omega), \tag{5}$$

where $\chi''(k,\omega)$ is the imaginary part of $\chi(k,\omega)$. This completes the MF formalism in general. For further details we refer to the review article by Yoshida and Takeno.[14]

We are now in a position to apply the above method to calculate $S(k,\omega)$ of a 2DEG. The starting point is to choose a reference system and the system of noninteracting electrons is the most obvious choice as it enables us to explicitly take into account the single-particle aspects of the dynamics and the statistics obeyed by the particles. Using the expressions for the frequency moments[15] in Eq. (3), we have

$$\alpha=1,\quad V_0=1/\chi(k)-1/\chi^{(0)}(k),$$

and

$$V_1=3[\langle K\rangle-\langle K\rangle^{(0)}]+(m/k^2)\omega_1^2(k)-V_0. \tag{6}$$

In the above equation $\chi(k)=-\chi(k,\omega=0)$ is the isothermal susceptibility of the interacting electron gas, $\langle K\rangle$ is the average kinetic energy per electron, and $\omega_1^2(k)$ is defined by

$$\omega_1^2(k)=\omega_p^2(k)[1-I(k)], \tag{7}$$

where $\omega_p(k)=(2\pi ne^2k/m)^{1/2}$ is the 2D plasmon frequency and $I(k)$ is given by

$$I(k)=\frac{1}{2k}\int_0^\infty\frac{dr}{r^2}[g(r)-1][1-J_0(kr)-3J_2(kr)]. \tag{8}$$

Here, $J_n(x)$ is the nth order Bessel function of the first kind and $g(r)$ is the electron pair-correlation function. From Eqs. (1), (2), and (6) we see that the calculation of $S(k,\omega)$ requires $\chi(k)$, $\langle K\rangle$, and $g(r)$ as inputs. We obtain these from the recent QMC calculations of Tanatar and Ceperley[12] and Moroni *et al.*[13] $\chi^{(0)}(k,\omega)$ is known due to Stern.[16] Thus, the calculation of $S(k,\omega)$ now reduces to the calculation of the interacting part of the second order MF $R_2(k,t)$. We use the Gaussian anastz for $R_2(k,t)$ in the same way as that used by Tanatar, i.e.,

$$R_2(k,t)=\exp[-\omega_d^2(k)t^2/2], \tag{9}$$

where $\omega_d(k)$ is the relaxation frequency related to the time decay of the MF. The Laplace transform $R_2(k,z)$ of $R_2(k,t)$ is defined as

$$R_2(k,z)=i\int_0^\infty dt\,e^{-izt}R_2(k,t), \tag{10}$$

where $z=\omega-i\varepsilon$, is the complex frequency. It may be noted that

$$R_2(k,\omega)=\lim_{\varepsilon\to0}R_2(k,z)=R_2'(k,\omega)+i\pi R_2''(k,\omega), \tag{11}$$

where $R_2'(k,\omega)$ and $R_2''(k,\omega)$ are the real and imaginary parts of $R_2(k,\omega)$. It is easy to show that

$$R_2'(k,\omega)=\frac{1}{\omega_d(k)}\exp\left(-\frac{\omega^2}{2\omega_d^2(k)}\right)\int_0^{[\omega/\omega_d(k)]}dx'\exp[x'^2/2] \tag{12a}$$

and

$$R_2''(k,\omega)=\frac{1}{\sqrt{2\pi}\omega_d(k)}\exp\left(-\frac{\omega^2}{2\omega_d^2(k)}\right). \tag{12b}$$

In the next section we present the results for $S(k,\omega)$ at different k for $r_s=1$ and 5. r_s is the dimensionless parameter describing the areal density n of electrons $[r_s=1/(a_B\sqrt{n\pi})$, where a_B is the Bohr atomic radius].

III. RESULTS AND DISCUSSION

In numerical calculations we choose a system of units where wave vector and frequency are expressed, respectively, in units of the Fermi wave vector k_F and the Fermi energy ε_F, distances in units of k_F^{-1} and energies in rydbergs (1 Ry$=e^2/2a_B$). The static inputs required are taken from the QMC calculation. The parameter $\omega_d(k)$ is adjusted so as to satisfy the zeroth sum rule of $S(k,\omega)$ to a good accuracy. The f-sum rule and the third sum rule are automatically satisfied in the present formalism independent of the choice of $\omega_d(k)$. In Fig. 1 we plot $S(k,\omega)$ at $k=1.593$

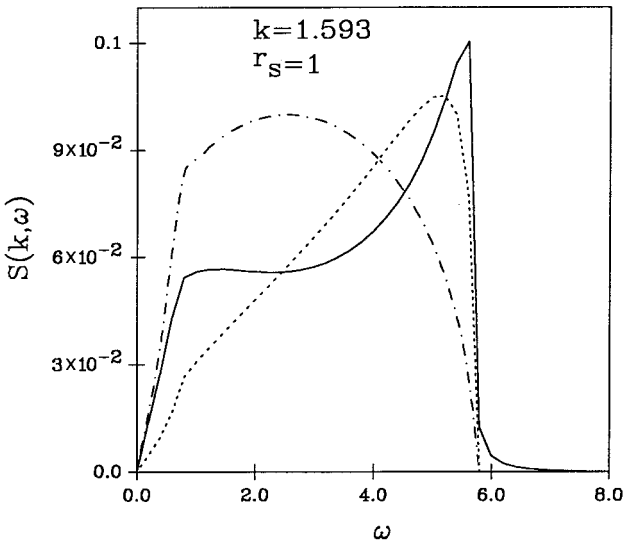

FIG. 1. The dynamic structure factor $S(k,\omega)$ vs ω at $k=1.593$, $r_s=1$, and $\omega_d=2.61$. Present $S(k,\omega)$ (solid line); $S^{(0)}(k,\omega)$ (dash-dot line); $S_{\mathrm{RPA}}(k,\omega)$ (dashed line).

and $r_s=1$ with $\omega_d=2.61$. The zeroth sum rule is satisfied within an error of about 6%. For comparison the noninteracting $S^{(0)}(k,\omega)$ and that obtained in the random-phase approximation (RPA) $S_{\mathrm{RPA}}(k,\omega)$ are also shown in Fig. 1. It is seen from Fig. 1 that $S(k,\omega)$ calculated in the above-described MF formalism shows a double-peak structure in contrast to the $S_{\mathrm{RPA}}(k,\omega)$ and the findings of Tanatar.[8] We have found that the line shape of $S(k,\omega)$, especially, its double-peak behavior, depends upon the choice of $\omega_d(k)$. To show the nature of dependence of $S(k,\omega)$ on $\omega_d(k)$ we plot it in Fig. 2 at $k=1.863$ and $r_s=1$ for three different choices of ω_d, namely, 2.91, 3.50, and 6.91. In Table I we give the dependence of the zeroth moment of $S(k,\omega)$ on $\omega_d(k)$ along with the QMC values of $S(k)$. It can be noticed from Fig. 2

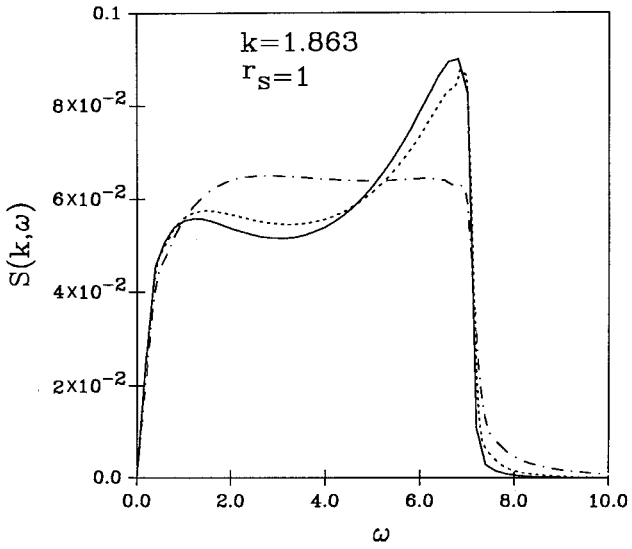

FIG. 2. The dynamic structure factor $S(k,\omega)$ vs ω at $k=1.863$, $r_s=1$. $\omega_d=2.91$ (solid line); $\omega_d=3.50$ (dashed line); $\omega_d=6.91$ (dash-dot line).

TABLE I. Dependence of zeroth moment of $S(k,\omega)$ on $\omega_d(k)$.

k	r_s	$\omega_d(k)$	$S(k)$	$S_{\mathrm{QMC}}(k)$	Percentage error
1.593	1.0	2.61	0.753	0.799	5.7%
1.863	1.0	2.91	0.851	0.905	5.9%
1.863	1.0	3.50	0.859	0.905	5.0%
1.863	1.0	6.91	0.887	0.905	2.0%
2.350	1.0	6.91	0.959	0.982	2.0%
2.100	5.0	13.5	0.896	0.909	1.4%

that the double-peak structure almost disappears at $\omega_d=6.91$ where the zeroth sum rule is satisfied with maximum accuracy among the cases investigated here. We have further found that by choosing $\omega_d>6.91$ the sum rule accuracy does not vary much and $S(k,\omega)$ shows only a single broad peak. A similar type of $S(k,\omega)$ dependence on ω_d is noted at $k=1.593$. However, at $k=2.35$ and $r_s=1$ with $\omega_d=6.91$, it is found that $S(k,\omega)$ shows a clear double-peak structure (plotted as a solid line in Fig. 3) with the zeroth sum rule condition satisfied within an acceptable error of 2%. This seems to suggest that at $r_s=1$ it is less probable to find a two-peak structure in $S(k,\omega)$ for $k\leqslant 1.863$ than at $k=2.35$. In order to see the effect of increasing r_s on the behavior of $S(k,\omega)$ we calculate it at $k=2.1$ and $r_s=5$ with $\omega_d=13.5$. The calculated $S(k,\omega)$ exhibits a pronounced double-peak structure and is shown by a solid line in Fig. 4. We also note from Table I that the sum rule criterion is satisfied to a very good accuracy. From the above discussion it can be concluded that the MF formalism used by us yields $S(k,\omega)$ that shows a clear double-peak structure at intermediate k at both $r_s=1$ and 5. This result is contrary to the prediction of Tanatar,[8] where $S(k,\omega)$ shows only a single broad peak at both $r_s=1$ and 5. Our calculation differs from that of Tanatar in the input used for $\chi(k)$. We have obtained

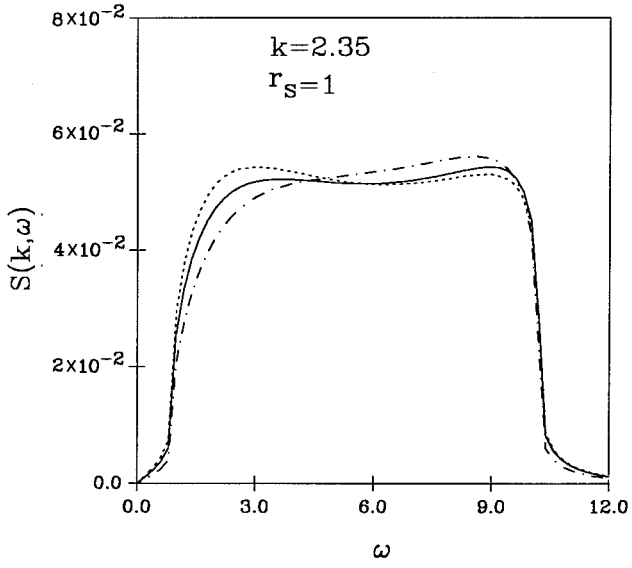

FIG. 3. The dynamic structure factor $S(k,\omega)$ vs ω at $k=2.35$, $r_s=1$, and $\omega_d=6.91$. Present $S(k,\omega)$ (solid line); $S_M(k,\omega)$ with $a(k)=b(k)=1.2$ (dashed line); $S_M(k,\omega)$ with $a(k)=0.8$, $b(K)=1.2$ (dash-dot line).

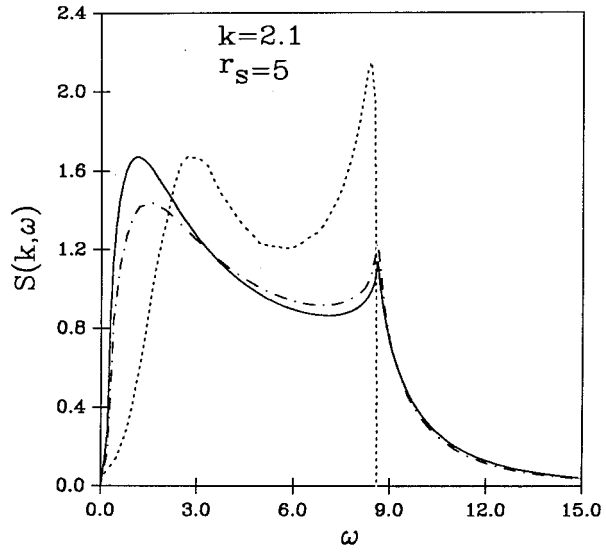

FIG. 4. The dynamic structure factor $S(k,\omega)$ vs ω at $k=2.1$, $r_s=5$, and $\omega_d=13.5$. Present $S(k,\omega)$ (solid line); $S_M(k,\omega)$ and $a(k)=1.0$, $b(k)=1.2$ (dash-dot line); $S_{\mathrm{QSTLS}}(k,\omega)$ (dashed line).

$\chi(k)$ from the accurate QMC calculation whereas Tanatar has used it for a lower-bound approximation as $\chi_{\mathrm{LB}}(k)=2S^2(k)/\omega_k[\omega_k=\hbar^2k^2/2m]$; $S(k)$ was taken from the QMC calculation. Thus, contrary to what was expected by Tanatar, the $S(k,\omega)$ behavior changes drastically by using $\chi_{\mathrm{QMC}}(k)$ as input for $\chi(k)$ in the formalism. To make the difference between $\chi_{\mathrm{LB}}(k)$ and $\chi_{\mathrm{QMC}}(k)$ more transparent we plot them in Fig. 5 along with the RPA curve at $r_s=1$. We notice that $\chi_{\mathrm{LB}}(k)$ differs considerably from $\chi_{\mathrm{QMC}}(k)$ and is rather close to $\chi_{\mathrm{RPA}}(k)$. In particular $\chi_{\mathrm{LB}}(k)$ exhibits a peak at $k\approx1.5$, in which $\chi_{\mathrm{QMC}}(k)$ is at $k\approx2$. Here, it may be noted that $\chi(k)$ results obtained by us using the[17] STLS and[7] QSTLS theories also do not agree with $\chi_{\mathrm{LB}}(k)$, but are, rather, closer to the QMC calculation.

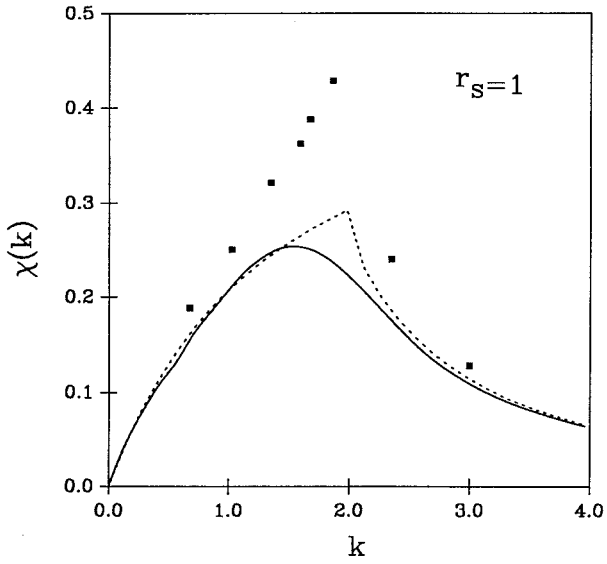

FIG. 5. The isothermal susceptibility $\chi(k)$ vs k at $r_s=1$. $\chi_{\mathrm{LB}}(k)$ (solid line); $\chi_{\mathrm{RPA}}(k)$ (dashed line); $\chi_{\mathrm{QMC}}(k)$ (solid squares).

To the best of our knowledge, there is neither simulation nor the experimental data available for $S(k,\omega)$ of a 2DEG to compare our results. Therefore, we compare our results with the other theories. For this we calculate $S(k,\omega)$ by using the parameterized model of Yoshida, Takeno, and Yasuhara,[11] where they approximate $V(k,\omega)$ by

$$V_M(k,\omega)=(m/k^2)[1-a(k)]\omega_p^2(k)+(m/k^2)\times[b(k)-1+a(k)]\omega_p^2(k)\omega R_2(k,\omega). \quad (13)$$

By using the Gaussian model for $R_2(k,t)$ and adjusting the parameters $a(k)$, $b(k)$, and $\omega_d(k)$ to satisfy the zeroth sum rule to a good accuracy, the authors in Ref. 11 obtained satisfactory results for $S(k,\omega)$ of a 3DEG. Following the same procedure, we calculate $S_M(k,\omega)$ at $k=2.35$ and $r_s=1$ and the result is shown as a dashed line in Fig. 3. The zeroth sum rule condition is satisfied within an accuracy of better than 1% for $a(k)=b(k)=1.2$ and $\omega_d=6.91$. It may be noted from Fig. 3 that $S_M(k,\omega)$ is fairly close to the present $S(k,\omega)$ and its qualitative behavior is similar to the 3D calculation of Yoshida *et al.*[11] Like the 3D case it is also found that its line shape is sensitive to the choice of $a(k)$ and $b(k)$. For example, $S_M(k,\omega)$ calculated with the same ω_d ($\omega_d=6.91$) but for $a(k)=0.8$, $b(k)=1.2$ is shown as a dash-dot line in Fig. 3. $S_M(k,\omega)$ is also calculated at $r_s=5$ and $k=2.1$ with $\omega_d=13.5$, $a(k)=1$, and $b(k)=1.2$. $S_M(k,\omega)$ thus obtained exhibits a double peak having its close resemblance with that calculated by using the present MF approach and is plotted as a dash-dot line in Fig. 4. Thus the model calculation based on the method of Yoshida *et al.* supports our prediction of finding a double-peak structure in $S(k,\omega)$ at intermediate k at both $r_s=1$ and 5.

We finally compare $S(k,\omega)$ with our recent result,[7] which we have obtained by using the QSTLS theory. From the comparative study we find that $S(k,\omega)$ differs both qualitatively and quantitatively from $S_{\mathrm{QSTLS}}(k,\omega)$ at $r_s=1$ while a qualitative similarity is noted at $r_s=5$. As a major difference we note that in QSTLS the double-peak structure is pronounced only at $r_s=5$ while in the present MF formalism it is pronounced at both $r_s=1$ and 5. In Fig. 4 $S_{\mathrm{QSTLS}}(k,\omega)$ at $k=2.1$ and $r_s=5$ is plotted as a dashed line. From the present and earlier investigations it seems that there is a good possibility of finding the two-peak structure in $S(k,\omega)$ of a 2DEG. Here, it may be noted that the double-peak structure of $S(k,\omega)$ in the present study is a property of the 2D electron system as no lattice effects are taken into account. A similar conclusion has been drawn in 3D by Mukhopadhyay, Kalia, and Singwi and others.[4] However, experiments by Schülke *et al.*[18] on 3D electron system in Li and Be metals, which are certainly not free-electron-like systems, atrributed the double-peak structure to the lattice effects. Since no experiment has been done so far to study $S(k,\omega)$ in 2D, the accuracy of any theory in predicting its line shape and the reason for the existence of the double peak in it cannot be known at present.

IV. CONCLUSIONS

The dynamic structure factor $S(k,\omega)$ of a 2DEG is calculated in the Mori memory function formalism by using the Gaussian model for the interacting part of the second-order memory function. The static inputs needed are obtained from the recent quantum Monte Carlo calculation. $S(k,\omega)$ thus obtained shows a clear two-peak structure at intermediate k at both $r_s=1$ and 5. Our results suggest that there is a good possibility of finding the double-peak structure in the experimental $S(k,\omega)$ at intermediate k in the 2D electron systems also.

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