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ABSTRACT

We evaluate the ground state properties of a charged Bose gas at $T = 0$ within the quantum version of the self-consistent field approximation of Singwi, Tosi, Land and Sjölander (STLS). The dynamical nature of the local field correction is retained to include dynamic correlation effects. The resulting static structure factor $S(q)$ and the local field factor $G(q)$ exhibit properties not described by other mean-field theories.

I. INTRODUCTION

The homogeneous gas of electrons interacting via the Coulomb potential is a useful model¹ to understand a vast range of physical phenomena. The continuing interest in this model stems partly from the realization of physical systems in the laboratory which lend themselves to such a description, and partly from theoretical reasons to understand the basic properties of a many-body system. Similarly, a system of charged particles obeying Bose statistics under the influence of Coulomb interactions is important in determining the effects of statistics and correlations in comparison with the electron gas. Charged bosons are the subject of renewed interest because of their possible role in some high-temperature superconducting systems² and in astrophysical applications.³

In the study of many-body properties of charged particles, the self-consistent field method of Singwi *et al.*⁴ (STLS) provides a means of going beyond the random-phase approximation (RPA) in a simple and physically motivated way. It has been successfully applied to electron gas systems in various situations including different dimensions^{4,5} and also to the charged Bose gas.^{6,7} The local field factor introduced in the STLS scheme to describe the correlation effects depends on the wave vector only. This is because classical distribution functions were used in its original derivation. A quantum version of the STLS approach (qSTLS) was developed by Hasegawa and Shimizu,⁸ which allows for a frequency dependent local field factor. A different formulation (with similar results) was put forward by Niklasson,⁹ who also elucidated the relations among various related approximations. Numerical calculations on the self-consistent equations for a three-dimensional (3D) electron gas were provided by Holas and Rahman.¹⁰ A detailed corresponding study in a 2D electron liquid has recently appeared.¹¹ Schweng *et al.*¹² have investigated the frequency dependence of $G(q, \omega)$ within a finite temperature formalism. The main finding of all these efforts has been that the quantum effects embodied in $G(q, \omega)$ change significantly the short-range correlations.

In this paper, we apply the qSTLS method to the study of a charged Bose gas in 3D. Our main motivation, apart from possible applications, is to test for charged bosons the efficiency

of the qSTLS method, which is demonstrated to yield accurate results for electron systems. We compare our results with more elaborate hypernetted chain (HNC) calculations¹³ and with quantal Monte Carlo (QMC) results.^{14,15} Both in the HNC calculations and in the QMC simulations static local field corrections have been extracted. In this work our aim is to investigate the dynamical nature of $G(q, \omega)$. The frequency dependence of the dynamic $G(q, \omega)$ has recently been emphasized in some theories dealing with superconductivity.¹⁶

The paper is organized as follows. In the next section we outline the qSTLS method. In Sec. III we present our self-consistent calculations, compare the results with other works and discuss the effects of $G(q, \omega)$ on certain physical quantities. We conclude with a brief summary in Sec. IV. In the Appendix, we provide some technical details on the calculation of $G(q, \omega)$.

II. THEORY

We consider a system of negatively charged bosons embedded in a uniform positive background, interacting via the Coulomb potential. The system is characterized by the dimensionless coupling constant $r_s = r_0/a_B$, where $r_0 = (3/4\pi n)^{1/3}$ is the average inter-particle spacing, $a_B = 1/me^2$ is the Bohr radius and n is the number density (we use $\hbar = 1$). The bare Coulomb interaction is given by $V(q) = 4\pi e^2/q^2$, and at the lowest order (in the Bogoliubov approximation) the static structure factor of the system is $S(q) = (1 + 2nV(q)/\epsilon_q)^{-1/2}$, where $\epsilon_q = q^2/2m$ is the free-particle energy. Using the Feynman expression for the excitation spectrum we can determine the collective modes of the system to be $\omega_{pl} = [\epsilon_q^2 + 2n\epsilon_q V(q)]^{1/2}$. The lowest order theory (also known as the uniform limit) neglects correlation effects, which become increasingly important at large coupling strength.

In the STLS approximation the density-density response function is given in the form of a generalized random-phase approximation (RPA),

$$\chi(q, \omega) = \frac{\chi_0(q, \omega)}{1 - V_{\text{eff}}(q, \omega) \chi_0(q, \omega)}, \quad (1)$$

where $\chi_0(q, \omega)$ is the zero-temperature dynamic susceptibility of a noninteracting Bose gas

$$\chi_0(q, \omega) = \frac{2n\epsilon_q}{(\omega + i\eta)^2 - \epsilon_q^2}, \quad (2)$$

defined in terms of the density n and free-particle energy ϵ_q (η is a positive infinitesimal quantity). The effective interaction $V_{\text{eff}}(q, \omega) = V(q)[1 - G(q, \omega)]$ is defined in terms of the dynamic (frequency dependent) local field factor

$$G(q, \omega) = -\frac{1}{n} \int \frac{d\mathbf{q}'}{(2\pi)^3} \frac{\chi_0(\mathbf{q}, \mathbf{q}'; \omega)}{\chi_0(q, \omega)} \frac{V(q')}{V(q)} [S(q - q') - 1], \quad (3)$$

for which we give an explicit formula in the Appendix. In the above expression for $G(q, \omega)$, the static structure factor $S(q)$ is related to the dynamical susceptibility through the fluctuation-dissipation theorem

$$S(q) = -\frac{1}{n\pi} \int_0^\infty d\omega \chi(q, i\omega), \quad (4)$$

where we have used the analytic continuation of the response function to the complex frequency plane followed by the Wick rotation of the frequency integral. This procedure is more effective in capturing the plasmon poles dominating the response of a Bose fluid.

The derivation leading to the expression for the frequency dependent local field factor $G(q, \omega)$ is similar to that in the static STLS approximation. Instead of using the classical distribution functions, a set of equations of motion for the Wigner distribution functions are considered. The hierarchy of coupled equations are terminated by making the assumption that the two-body Wigner distribution function may be written as a product of one-body distribution functions and the pair correlation function $g(r)$.^{8,10} The frequency dependence of $G(q, \omega)$ comes from the factors $\chi_0(\mathbf{q}, \mathbf{q}'; \omega)$ and $\chi_0(q, \omega)$ which are the inhomogeneous and homogeneous free-particle response functions, respectively. We give the definition of $\chi_0(\mathbf{q}, \mathbf{q}'; \omega)$ and a simple quadrature formula for $G(q, i\omega)$ (evaluated on the imaginary frequency axis) in the Appendix. We iterate between $G(q, i\omega)$ and $S(q)$, which uses $\chi(q, i\omega)$ and in turn $G(q, i\omega)$, until self-consistency is achieved.

It is known that the STLS approach fails to fulfill the compressibility sum-rule, namely the compressibility evaluated directly from the ground-state energy is not equal to that

calculated using the long-wavelength limit of $G(q, 0)$. This deficiency may be overcome within a construction given by Vashishta and Singwi¹⁷ and may be applied to the present problem of dynamic local field corrections as shown by Holas and Rahman.¹⁰ Since our primary aim is to investigate the qualitative effects of frequency dependence of $G(q, \omega)$, we consider only the qSTLS scheme.

III. RESULTS AND DISCUSSION

Since the dynamic local field factor depends on the static structure factor within the qSTLS approximation, and the latter depends on the former through the fluctuation-dissipation integral, they have to be calculated self-consistently. Although the frequency dependence of $G(q, \omega)$ makes the calculation slightly more demanding than the usual STLS method,^{6,7} it is still manageable and we performed calculations for several densities until convergence was achieved to an accuracy of 0.01%.

We first discuss the static structure factor resulting from our self-consistent calculations. The static structure factor of the 3D charged Bose system is shown in Fig. 1, for various r_s values. The correlation effects (treated here dynamically) induce a vast difference with increasing r_s , compared to the RPA results (when $G(q, \omega) = 0$) and the static STLS results.⁶ At high densities (small r_s) $S(q)$ is similar to that obtained within the static STLS approximation.^{6,7} As r_s increases a peak structure starts to appear with increasing amplitude. Such peaks in the static structure factor were observed in the calculations of Apaja *et al.*¹³ in which the hypernetted-chain approximation was used, and in the Monte Carlo simulations of Moroni *et al.*¹⁵ We attribute the peak structure in $S(q)$ to the inclusion of dynamic correlation effects. The static STLS calculations of Conti *et al.*⁷ also show the emergence of a peak in $S(q)$ at large r_s , when the self-consistency condition on the compressibility sum-rule is imposed.

In Fig. 2 the probability of finding a particle at distance r away from a particle situated at the origin, namely the pair distribution function $g(r)$ is shown for several r_s values. We

use the Fourier transform

$$g(r) = 1 + \frac{1}{2\pi^2 nr} \int_0^\infty dk k \sin(kr) [S(k) - 1] \quad (5)$$

to find that $g(r)$ remains positive for $r_s \lesssim 12$. This is a large improvement over the RPA (or Bogoliubov) result. The $g(r)$ within the present qSTLS approach starts to become negative for small values of r as the coupling strength increases. We point out, however, that in the present scheme only the dynamics of the Pauli correlation hole is taken into account, but not the Coulomb correlation hole which becomes dominant at low densities.¹¹

From our self-consistent calculations of the correlation effects we obtain the frequency dependent local field factor. Fig. 3 shows $G(q, i\omega)$ as a function of frequency on the imaginary axis. We note that $G(q, i\omega)$ is a smooth function of ω , tending to a constant for fixed values of q , and most of the frequency dependence is confined to the low frequency region. The QMC simulations can only reveal information on the static local field, thus our frequency dependent results for $G(q, \omega)$ present a different aspect of the correlation effects.

The real and imaginary parts of $G(q, \omega)$ may be obtained from $G(q, i\omega)$ by the analytic continuation $i\omega \rightarrow \omega + i\eta$ in Eq. (3). We show in Fig. 4 the real and imaginary parts of $G(q, \omega)$ as functions of frequency at $r_s = 10$ and $qr_0 = 2, 4$ and 6 . We observe that both the real and imaginary parts of $G(q, \omega)$ oscillate as a function of ω . One can show that for fixed q and large ω , the local field factor behaves as

$$\lim_{\omega \rightarrow \infty} G(q, \omega) = G_{\text{STLS}}(q) + \mathcal{O}(1/\omega^2), \quad (6)$$

a property also known to exist in electron fluids.¹⁰ Thus, $\text{Im}[G(q, \omega)]$ vanishes and $\text{Re}[G(q, \omega)]$ tends to the value given by the static STLS approximation for large ω , as illustrated in Fig. 4. In the static limit, i.e. $\omega = 0$, $\text{Im}[G(q, 0)]$ vanishes, and the real part satisfies $\lim_{q \rightarrow \infty} G(q, 0) = 1 - g(0)$.

The zero-frequency limit $G(q, 0)$ is of interest in most practical applications. Within the dynamical STLS theory $G(q, 0)$ is given by

$$G(q, 0) = \frac{q^3}{3\pi} \int_0^\infty dk \frac{k}{(q^2 - k^2)} \ln \left| \frac{q - k}{q + k} \right| [S(k) - 1]. \quad (7)$$

In Fig. 5 we employ the above expression using our self-consistent $S(q)$ (solid lines) and that coming from the QMC simulations¹⁵ (dashed lines). We observe that both calculations agree quantitatively for $qr_0 \lesssim 2$ and qualitatively for $qr_0 \gtrsim 2$. The differences originate from the respective structure factors. $G(q, 0)$ calculated in this manner is very different from the results of static STLS approximation⁶ and also from $G(q)$ of QMC simulations.¹⁵ We note that in the QMC simulations $G(q)$ is evaluated directly by the response of the system to an external perturbation, without using the static structure factor $S(q)$. It remains interesting that $G(q, 0)$ for charged bosons displays rather different behavior than the QMC results, whereas in the electron gas case¹⁰ it provides a meaningful estimate.

The high-frequency limit of our $G(q, \omega)$ also yields a frequency independent local field factor $G_\infty(q)$. Our self-consistent results for $G_\infty(q)$ are compared with the QMC and static STLS approximations in Fig. 6. We observe in Fig. 6 that the qSTLS approximates the local field factor at small q , but is not able to reproduce the large q behavior of the QMC results. This is not surprising since the large- q nature of $G(q)$ mainly comes from the momentum-distribution (or kinetic energy of the interacting system), which we have assumed to be a δ -function. However, our results capture part of the essential features seen in the more precise theories.^{13,15} For instance, the peak structure in $G_\infty(q)$ can be identified as in the QMC and HNC calculations around $qr_0 \approx 4$, where the first star of the reciprocal lattice of the body-centered cubic crystal would lie. STLS-type mean-field theories without the frequency dependence⁶ tend to display a monotonic behavior in $G(q)$. Thus, it appears that our $G_\infty(q)$ may be useful as a good estimate of the true $G(q, 0)$, i.e. as extracted from QMC simulations.

In Fig. 7 we plot the plasmon dispersion curve ω_q scaled with the long-wavelength plasmon energy $\omega_{pl} = (12r_s)^{1/2}$ at various r_s values. ω_q is obtained by solving for the pole of the dynamic susceptibility given in Eq. (1), which includes the frequency dependent local field factor. We compare our results with the plasmon dispersion in the RPA [$\omega_q^{\text{RPA}} = (12r_s)^{1/2}(1 + q^4/12r_s)^{1/2}$] and with the static STLS calculations.⁶ For small q , the

plasmon dispersion obtained from the present dynamical theory is very similar to that of static STLS. The roton minimum appearing at intermediate q , on the other hand, is more pronounced and shifted towards the low- q side. At large q the qSTLS results approach the RPA faster than the static STLS. The differences between the qSTLS and the static STLS approximations become more marked with increasing r_s . Since our frequency-dependent local field factor has an imaginary part, we also calculate the damping γ_q , of the plasma excitations by solving for the imaginary part of the equation

$$1 - V(q)[1 - G(q, \omega_q - i\gamma_q)]\chi_0(q, \omega_q - i\gamma_q) = 0. \quad (8)$$

Carrying out a standard analysis¹⁸ which assumes that $\gamma_q \ll \omega_q$, we find that the damping is given by

$$\gamma_q = \frac{(1 - \text{Re}[G])\text{Im}[\chi_0] - \text{Im}[G]\text{Re}[\chi_0]}{(1 - \text{Re}[G])\frac{\partial \text{Re}[\chi_0]}{\partial \omega} - \text{Re}[\chi_0]\frac{\partial \text{Re}[G]}{\partial \omega}} \Bigg|_{\omega=\omega_q}. \quad (9)$$

γ_q calculated according to the above expression is of the order of $0.5 \times 10^{-3} \omega_{pl}$ for $qr_0 \lesssim 2.5$.

In general, the excitation spectrum of a charged Bose gas contains multipair excitations¹ in addition to the plasmon mode. Our approach neglects multiparticle correlation effects since the lowest order polarization diagram described by $\chi_0(q, \omega)$ is included in the calculation of $G(q, \omega)$. The role of multiparticle effects in the excitation spectrum as described by the dynamic structure factor $S(q, \omega)$ has been thoroughly discussed by Apaja *et al.*¹³

It has been argued^{19,10} that when the static local field factor $G(q, 0)$ becomes greater than unity, the system of charged particles may exhibit the formation of a charge density wave (CDW). The instability will set in at a critical r_s value when

$$G(q, 0) = 1 + \frac{1}{V(q)|\chi_0(q, 0)|}, \quad (10)$$

which may be derived from the condition $1/\epsilon(q, 0) \leq 1$, for the static dielectric function. Since the accurate QMC results^{14,15} show no evidence of the violation of the above inequality, it may be concluded that the charged bosons remain in a stable fluid phase till crystallization occurs.

We have uncritically assumed that the charged Bose gas is in the condensate state and determined the effects of correlations induced by Coulomb interaction, as in previous calculations of a similar nature.^{6,7} However, the QMC simulations¹⁵ indicate that even at relatively high density (weak coupling) only about 80% of the particles are in the condensate. The interactions enormously deplete the condensate so that by $r_s = 160$ (crystallization density), most of the particles occupy non-zero momentum states. Thus, the results of approximate theories such as STLS or qSTLS should be used with caution at large r_s values. It might be possible to account for the effects of the particles out of the condensate by choosing a suitable model for the distribution function (say, a Gaussian) that determines the response of the noninteracting system. These ideas need to be explored within the self-consistent scheme for quantitative assessment.

IV. SUMMARY

We have considered the system of charged bosons at $T = 0$ and studied the effects of interactions within the quantum version of the STLS scheme. The self-consistently calculated static structure factor $S(q)$ exhibits a peak around $qr_0 \approx 4$ with increasing r_s , in agreement with QMC and HNC calculations. The local field factor $G(q, \omega)$ is frequency dependent in the present approximation and reveals information about dynamical correlations. In particular, inclusion of the dynamic $G(q, \omega)$ improves the static STLS results in predicting the r_s -dependent behavior of $G(q)$ for wave vectors $qr_0 \lesssim 4$.

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APPENDIX A: QUADRATURE FORMULA FOR $G(q, i\omega)$

In this appendix we provide some details for obtaining a one-dimensional quadrature expression for $G(q, i\omega)$. The local field factor is evaluated for frequencies on the imaginary axis, which greatly simplifies the self-consistent calculations.

The response function for the noninteracting inhomogeneous system is defined by

$$\chi_0(\mathbf{q}, \mathbf{q}'; \omega) = \int d^3\mathbf{p} \frac{f(\mathbf{p} + \mathbf{q}'/2) - f(\mathbf{p} - \mathbf{q}'/2)}{\omega - \mathbf{p} \cdot \mathbf{q}/m + i\eta}, \quad (\text{A1})$$

which reduces to that of the homogeneous system, viz. $\chi_0(q, \omega)$, for $\mathbf{q} = \mathbf{q}'$. Taking the distribution function as $f(\mathbf{p}) = n\delta(\mathbf{p})$ for bosons at $T = 0$, we obtain

$$\chi_0(\mathbf{q}, \mathbf{q}'; \omega) = \frac{2n\epsilon_{q\mathbf{q}'}}{(\omega + i\eta)^2 - \epsilon_{q\mathbf{q}'}}^2, \quad (\text{A2})$$

where $\epsilon_{q\mathbf{q}'} = \mathbf{q} \cdot \mathbf{q}'/2m$. Starting from Eq. (3) and using the above expression for χ_0 , the angular integration for $G(q, i\omega)$ is evaluated as

$$\begin{aligned} & \int_{-1}^1 d\mu \frac{q^2 - qk\mu}{\omega^2 + (q^2 - qk\mu)^2} \frac{1}{q^2 + k^2 - 2kq\mu} \\ &= -\frac{1}{2qk(4\omega^2 + q^4 - 2q^2k^2 + k^4)} \left\{ 4\omega \left[\tan^{-1} \left(\frac{q(q-k)}{\omega} \right) - \tan^{-1} \left(\frac{q(q+k)}{\omega} \right) \right] \right. \\ & \quad \left. + (k^2 - q^2) \ln \left| \frac{\omega^2 + q^4 - 2q^3k + q^2k^2}{\omega^2 + q^4 + 2q^3k + q^2k^2} \right| + 2(q^2 - k^2) \ln \left(\frac{q-k}{q+k} \right)^2 \right\}, \end{aligned} \quad (\text{A3})$$

in which the momentum variables q and k are scaled with r_0 and the energy variable ω is scaled with $1/2mr_0^2$. Finally, the one-dimensional quadrature expression for $G(q, i\omega)$ takes the form

$$G(q, i\omega) = -\frac{1}{3\pi} (\omega^2 + q^4) \int_0^\infty dk k^2 P(k, q; \omega) [S(k) - 1], \quad (\text{A4})$$

where $P(k, q; \omega)$ is the result of the angular integral given by the right-hand-side of Eq. (A3).

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FIG. 1. (a) The static structure factor $S(q)$ in a charged Bose gas at $r_s = 1$. Solid and dotted lines show the qSTLS and RPA results, respectively. Crosses are the QMC simulation results from Ref. 15. (b)-(d) $S(q)$ at $r_s = 5, 10$ and 20 , respectively. In (b)-(d) the dashed lines are the static STLS results from Ref. 6.

FIG. 2. (a) The pair-correlation function $g(r)$ as a function of r . Curves from top to bottom are for $r_s = 1, 5$ and 7 , respectively. Dotted lines are the RPA results. (b) $g(r)$ at lower density. Curves from top to bottom as they appear on the ordinate indicate $r_s = 10, 20, 30$ and 50 , respectively.

FIG. 3. (a) The local field factor evaluated on the imaginary frequency axis as a function of ω (in units of $1/2mr_0^2$) at (a) $r_s = 1$ and (b) $r_s = 5$. Dotted, dashed and solid lines are for $qr_0 = 2, 4$ and 6 , respectively.

FIG. 4. (a) The real part of $G(q, \omega)$ as a function of frequency at $r_s = 10$ and $qr_0 = 2$ (dotted line), $qr_0 = 4$ (dashed line), and $qr_0 = 6$ (solid line). (b) Same as (a) for the imaginary part of $G(q, \omega)$.

FIG. 5. (a)-(d) The local field factor $G(q, 0)$ at $r_s = 1, 5, 10$ and 20 , calculated within the dynamical theory with self-consistent $S(q)$ (solid lines) and QMC- $S(q)$ (dashed lines).

FIG. 6. $G(q)$ in various approximations. Crosses, open circles and solid circles indicate the QMC $G(q)$ at $r_s = 10, 20$ and 50 , respectively. Solid lines are the present results of $G(q, \omega = \infty)$ from bottom to top at the same r_s values. Dotted lines are the static STLS results of Ref. 6.

FIG. 7. The plasmon dispersion relation ω_q scaled with respect to the long-wavelength plasmon energy as a function of q . Solid curves from top to bottom are for $r_s = 5, 10$ and 20 , respectively. Dashed and dotted lines are the corresponding results of the static STLS approximation from Ref. 6 and of the RPA, respectively.

Figure 1

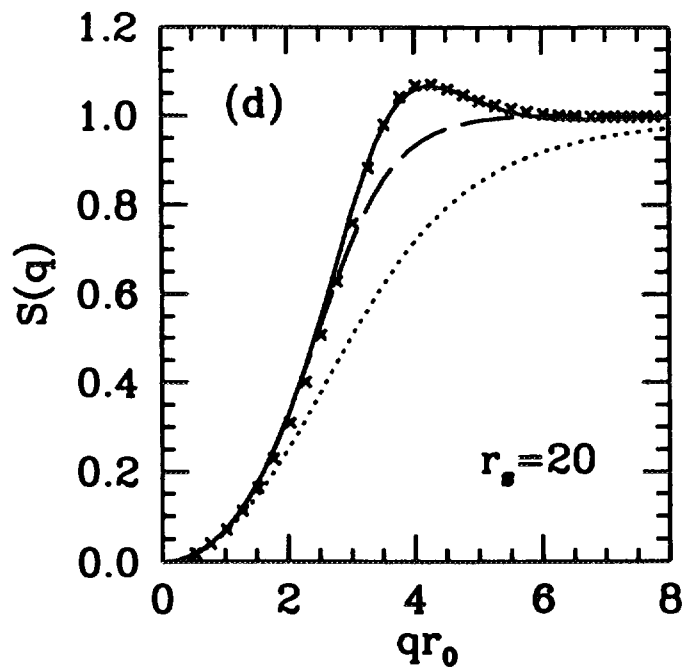
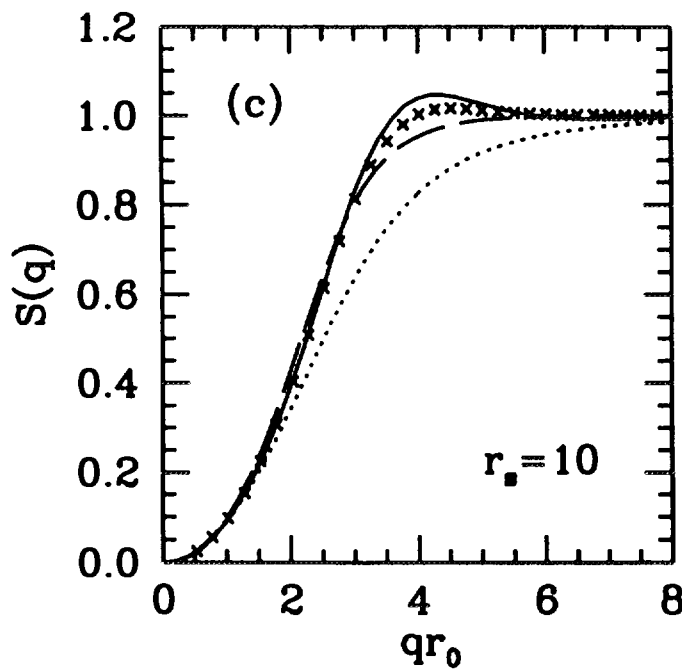
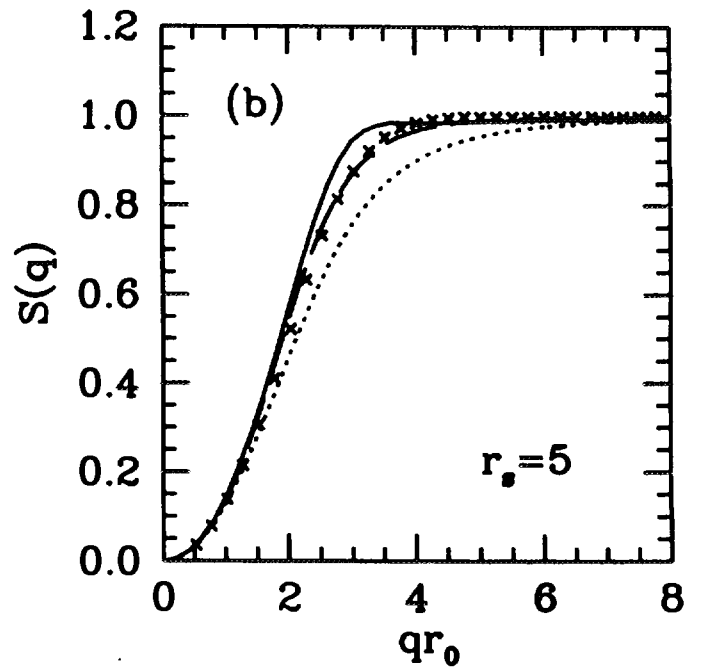
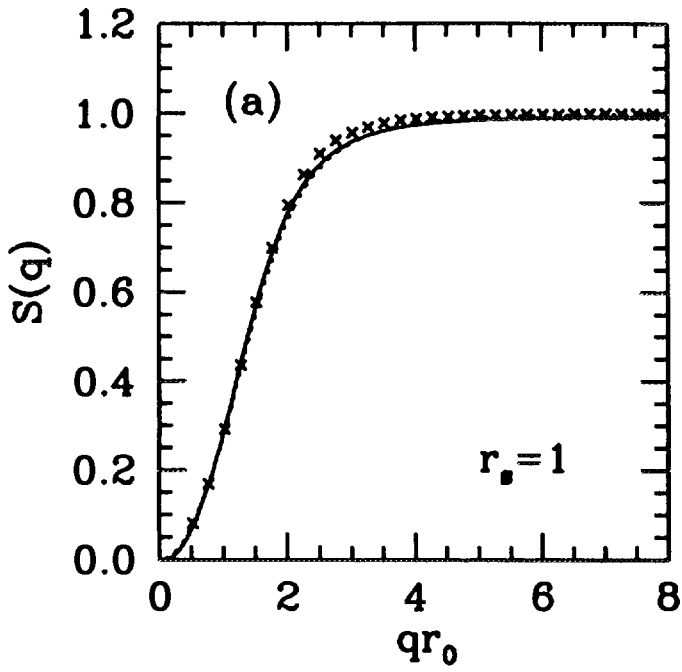


Figure 2

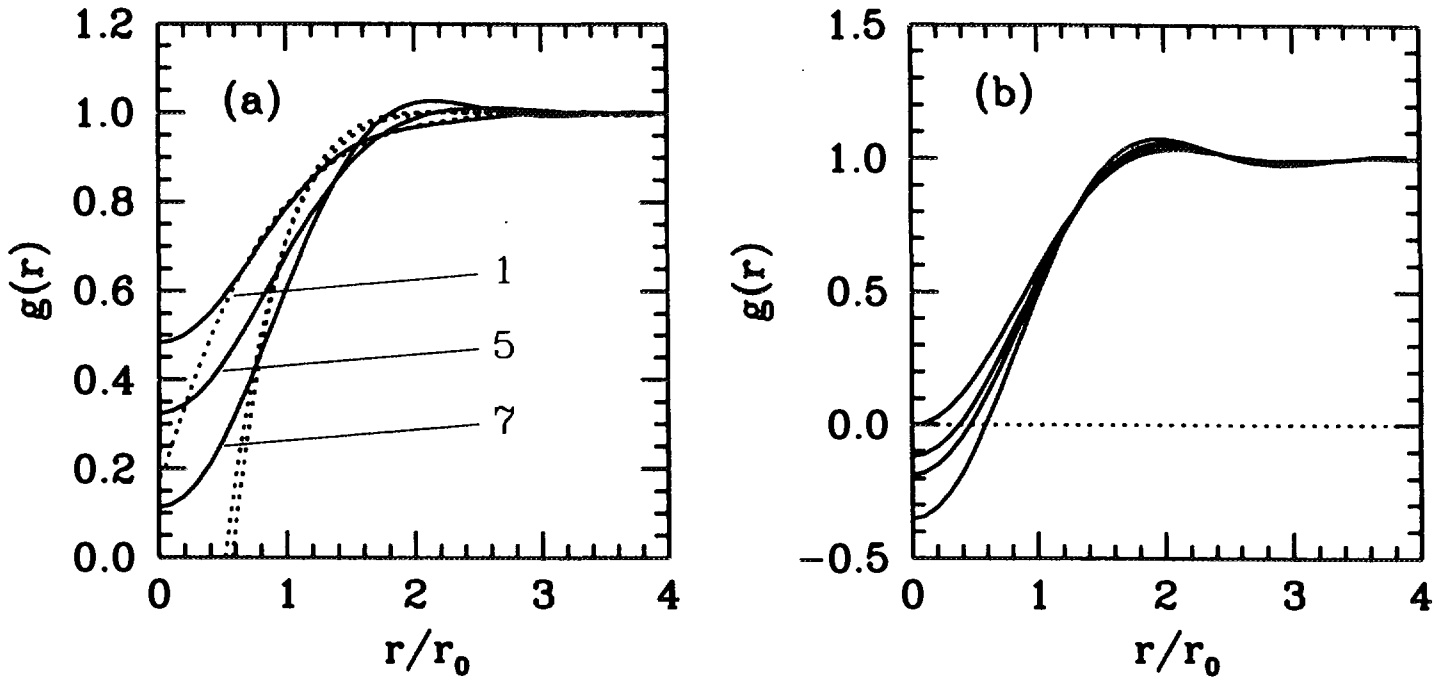


Figure 3

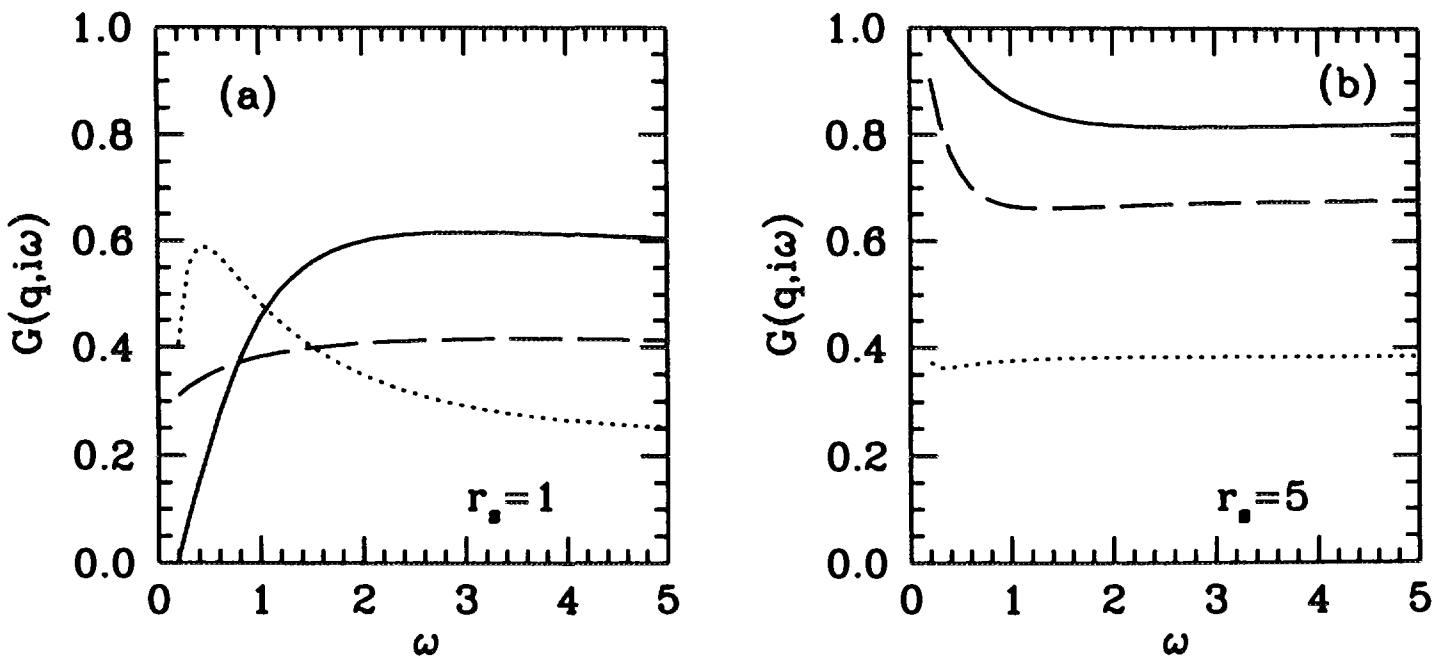


Figure 4

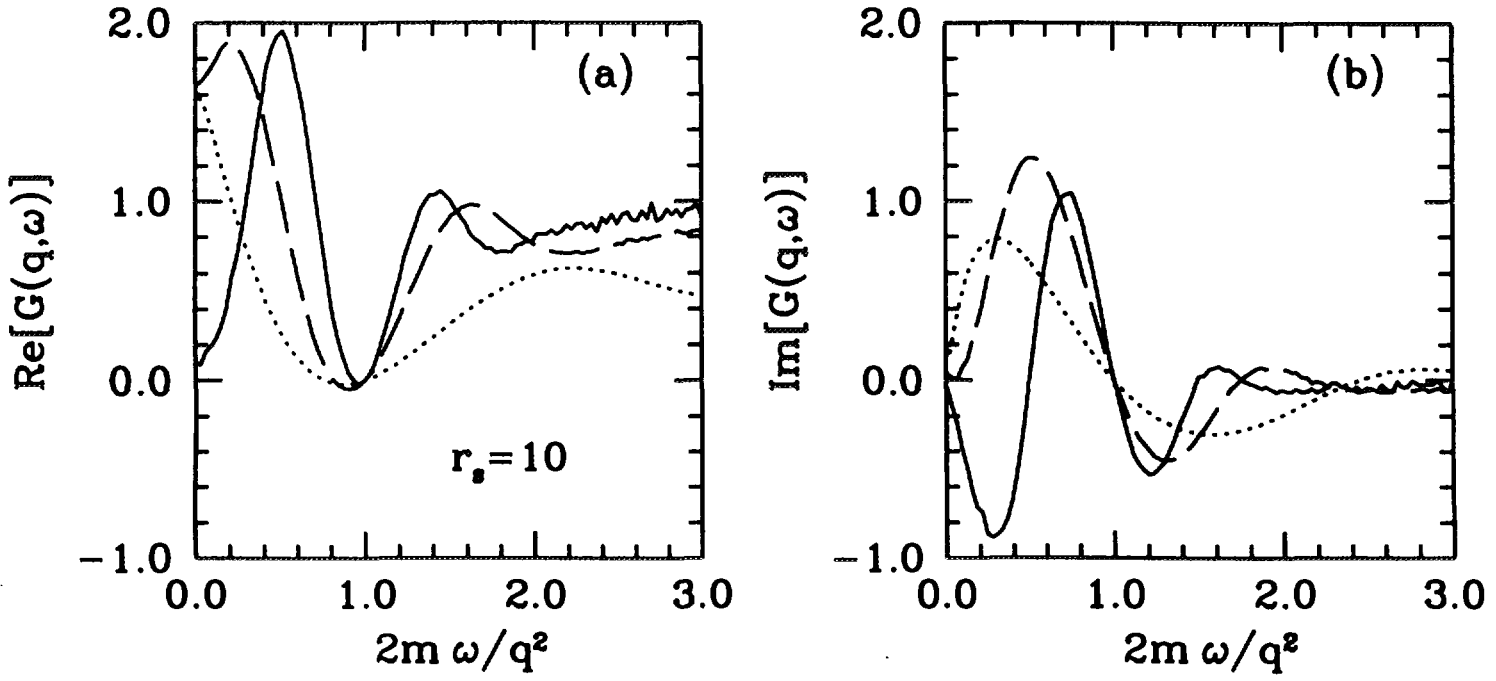


Figure 6

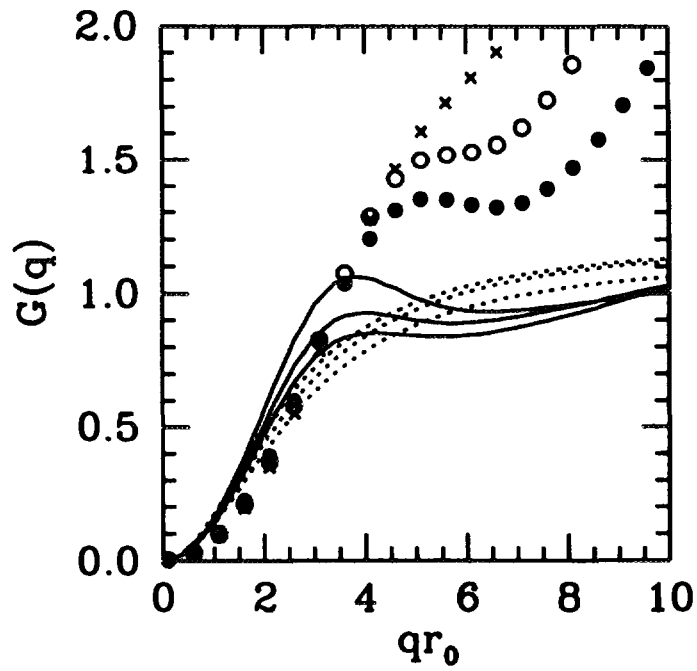


Figure 5

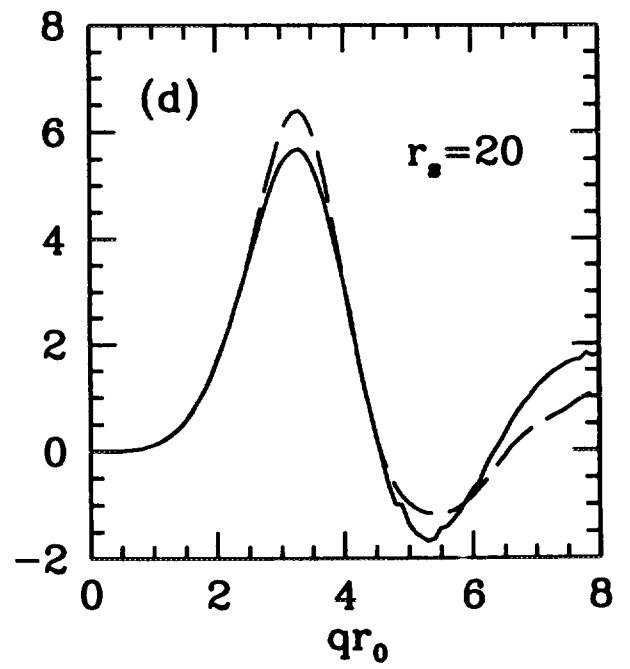
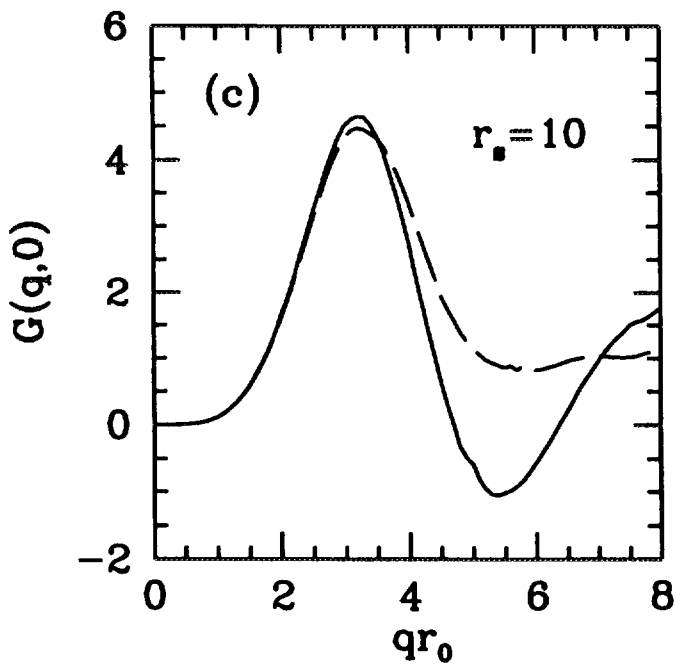
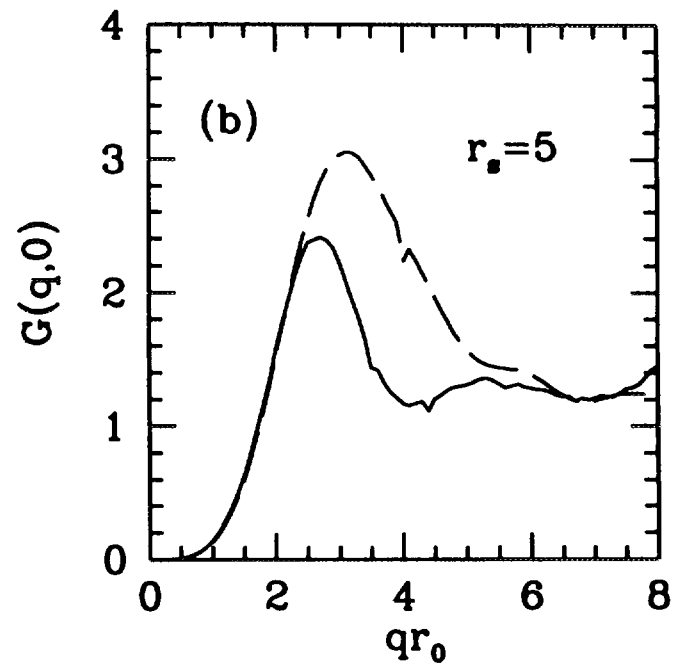
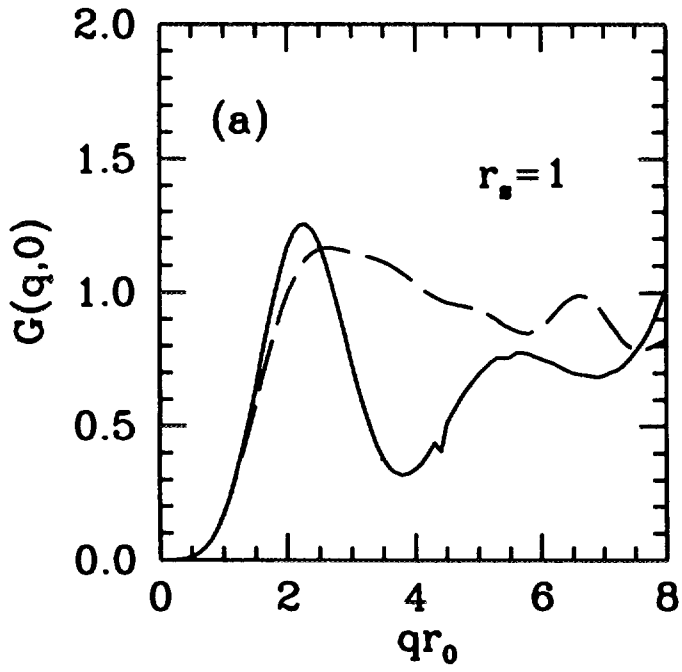


Figure 7

