Van Hove correlation functions for identical fermions: Effects of interactions

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The self-part of the dynamic structure factor for three-dimensional jellium is investigated within first-order perturbation theory. It is shown that using a screened Thomas-Fermi potential instead of the pure Coulomb interaction significantly reduces the breakdown range of the model to approximately $q \ll \sqrt{r_s} k_f$.

I. INTRODUCTION

An important concept in the classical many-body theory is the self-motion of a particle, leading immediately to the *self* and *distinct* structure factors. These functions, originally introduced by Van Hove,[1] are defined as the probability of finding the *same* or *two different* particles, respectively, at given locations and times. In the paper by Macke *et al.*[2] some important basic properties of the Van Hove functions in a fermion system have been pointed out clearly: They are violating the detailed balance and hence it is not straightforward to see how they can be calculated within the framework of one of the well-established approximations, e.g., random-phase approximation (RPA) or STLS.[3,4] Consequently, the authors of Ref. 2 have used an equation-of-motion method to go beyond the interaction free case. Based on calculations by Gasser[5] and Bachlechner, Miesenböck, and Macke,[6] they developed a second-order theory for $\chi^d(q,\omega)$, the distinct part of the dynamic susceptibility. For the pure self-structure factor $S^s(q,\omega)$, however, no interaction effects were considered although especially this function might be of great importance for constructing a generalization of Kerr's formula.[7]

In the present paper we first investigate $S^s(q,\omega)$ for an interacting Fermi gas in first-order perturbation theory. The result does not only show the well-known discontinuities at characteristic frequencies, but also an obvious breakdown of the approximation occurs already for $q \lesssim 2k_f$. To overcome this problem we then reevaluate the first-order formula with a screened Thomas-Fermi potential instead of the pure Coulomb interaction which significantly defers the breakdown of the model to approximately $q \ll \sqrt{r_s} k_f$. A brief discussion of the results ends this paper.

II. $S^s(q,\omega)$ IN FIRST-ORDER THEORY

Writing down the dynamic structure factor and its distinct part in field quantization[2] ($N \gg 1$)

$$S(q,t) = \frac{1}{N} \sum_{\mathbf{k},\mathbf{k}'} \langle c^\dagger_{\mathbf{k},t} c_{\mathbf{k}+\mathbf{q},t} c^\dagger_{\mathbf{k}'} c_{\mathbf{k}'-\mathbf{q}} \rangle - N\delta_{\mathbf{q},0} ,$$
$$S^d(q,t) = \frac{1}{N} \sum_{\mathbf{k},\mathbf{k}'} \langle c^\dagger_{\mathbf{k},t} c^\dagger_{\mathbf{k}'-\mathbf{q}} c_{\mathbf{k}'} c_{\mathbf{k}+\mathbf{q},t} \rangle - N\delta_{\mathbf{q},0} , \tag{1}$$

it is easily verified that

$$S(q,\omega) = S^d(q,\omega) + S^{s(0)}(q,\omega) + \Delta S^{s(1)}(q,\omega) + O(V^2) \tag{2}$$

with

$$\Delta S^{s(1)}(q,t) = \frac{1}{N} \sum_{\mathbf{k}} (\langle \Delta c^\dagger_{\mathbf{k},t} [\tilde{c}_{\mathbf{k}+\mathbf{q},t}, \rho_{-\mathbf{q}}] \rangle^0 + \langle c^\dagger_{\mathbf{k},t} [\Delta c_{\mathbf{k}+\mathbf{q},t}, \rho_{-\mathbf{q}}] \rangle^0) \tag{3}$$
$$\Delta c^{(\dagger)}_{\mathbf{k},t} \equiv c^{(\dagger)}_{\mathbf{k},t} - \tilde{c}^{(\dagger)}_{\mathbf{k},t} , \quad \rho_{\mathbf{q}} \equiv \sum_{\mathbf{k}} c^\dagger_{\mathbf{k}} c_{\mathbf{k}+\mathbf{q}} ,$$

where the tilde symbol on an operator is denoting its interaction representation. Using Dirac's perturbation expansion the time dependencies in Eq. (3) can be calculated for the ground-state jellium system up to first order of the interparticle potential V_q, yielding the main result,

$$\Delta S^{s(1)}(q,t) = \frac{1}{N} \sum_{\mathbf{k},\mathbf{p}} n_{\mathbf{k}} (n_{\mathbf{k}+\mathbf{p}} - n_{\mathbf{k}+\mathbf{p}+\mathbf{q}}) e^{-i(\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}})t} \left[(v_0 - v_p) it - (v_q - v_p) \frac{1 - e^{-i(\mathbf{p}\cdot\mathbf{q}/m)t}}{\mathbf{p}\cdot\mathbf{q}/m} \right] , \tag{4}$$

where $n_{\mathbf{k}}$ and $\varepsilon_{\mathbf{k}}$ are the free momentum distribution and the single-particle energy, respectively. The numerical evaluation of Eq. (4) follows, in principle, the methods used by Holas, Aravind, and Singwi[8] for the dynamic structure factor. Since the calculations are rather extensive only the final results will be presented here.

(i) The evaluation of the nonrenormalized $\Delta S^{s(1)}(q,\omega)$, i.e., the Fourier transform of Eq. (4) with v_q being the pure Coulomb potential, reveals two characteristic features. One observes jump discontinuities for arbitrary q at the characteristic frequencies $\omega_s = |q \pm q^2/2|$ which are similar to those described by Holas *et al.*[8] Additionally, the constant q scans for $q \lesssim 2k_f$ of $S^{s(1)}(q,\omega)$ show a dominating double-peak structure where the valley between the peaks is given by

$$\Delta S^{s(1)}(q,\omega=0) \underset{q\to 0}{\longrightarrow} -\frac{4\pi^2}{q^3} \tag{5}$$

as q reaches zero. Since the interaction free $S^{s(0)}(q,\omega=0)$ behaves like $+q^{-1}$ for small q, the $-q^3$ divergence

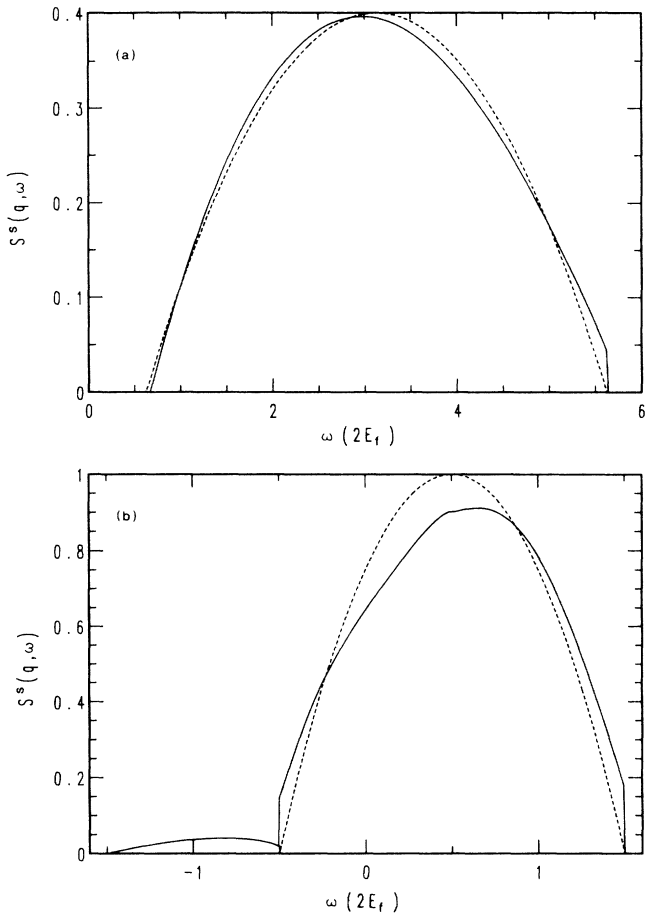

FIG. 1. The self-part of the dynamic structure factor in units of $mk_f/2n\pi$ at $r_s=2$ for a free-electron gas (dashed line) and calculated in the present first-order approximation (solid line). (a) $q=2.5k_f$, (b) $q=k_f$.

and the resulting double peak must be interpreted as a breakdown of the expansion.

(ii) Evaluating Eq. (4) with a Thomas-Fermi potential instead of the Coulomb interaction significantly improves these results: The height of the jump discontinuities is reduced and the first-order correction $\Delta S^{s(1)}(q,\omega=0)$ now shows the expected $q\rightarrow 0$ behavior proportional to q^{-1} (cf., Fig. 1). For q smaller than the Thomas-Fermi vector $q_{\rm TF}$, however, a double-peak structure is still arising, although again this is merely announcing the breakdown of the approximation. In the following conclusions some arguments for this interpretation will be given.

III. CONCLUSION

Starting with the well-known RPA result for the dynamic susceptibility

$$\chi(q,\omega)=\frac{\chi^0(q,\omega)}{1-v_q\chi^0(q,\omega)}\ , \tag{6}$$

one could, in principle, expand Eq. (6) to first order, yielding $\chi=\chi^0+v_q(\chi^0)^2$. Since $v_q\chi^0(q,\omega=0)^2$ is diverging like q^{-2} for $q\rightarrow 0$ a similar situation to that one described in case (i) of Sec. II is found. Noting that $1+v_{\rm TF}\chi^0\simeq(1-v\chi^0)^{-1}$ for $\omega=0$ and $q\rightarrow 0$, the method of case (ii) in Sec. II leads back to the renormalized χ of Eq. (6). From this example it is clear that a nonrenormalized perturbation expansion for the Coulomb interaction will always be restricted to small ranges of validity; it is, however, not guaranteed that the simple screening of the potential leads to a theory valid for all q and ω. There is indeed strong evidence that the double-peak structure is an artifact of the approximation, not a physical effect: The $q\rightarrow 0^+$ limit of $S^{s(1)}_{\rm TF}(q,\omega=0)$ does not interchange with the $r_s\rightarrow 0$ limit, i.e.,

$$\lim_{r_s\rightarrow 0}\lim_{q\rightarrow 0^+}\Delta S^{s(1)}(q,\omega=0)\neq 0\ .$$

Since this effect is also the mathematical origin of the double-peak structure that occurs for $q<q_{\rm TF}$ it is quite probably just announcing the breakdown of the approximation. Furthermore, the relevant terms for this behavior are proportional to v_q which is a direct analogy to the example discussed above.

Although the present approximation for $S^s(q,\omega)$ of an electron gas seems to provide useful results for $q>q_{\rm TF}$ and $\omega\neq\omega_s$ it will be an important task to improve this model using more refined theories. In any case, the Van Hove correlation functions turn out to represent an interesting as well as important approach to the dynamic aspects of a quantum many-particle system.

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