Asymptotically Exact Solution of the Dynamic Structure Factor of an Electron Gas at $r_s \approx 3.5$

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(Received 28 September 1992)

An analytic expression for the dynamic structure factor $S(k,\omega)$ of a 3D electron gas is obtained by the recurrence relation method. It is valid for one metallic density $r_s \approx 3.5$ and is exact asymptotically, i.e., $k \gg k_F$ (k_F the Fermi wave vector). The result is based on an assumption, justified by the kinetic-energy and static-structure-factor sum rules and also numerically approximately corroborated. The expression is compared with an experimental measurement of Li at $k = 2.08 k_F$.

PACS numbers: 71.45.−d, 05.30.Fk

Except possibly at the long wavelength limit, the dynamic structure factor $S(k,\omega)$ of a 3D electron gas at metallic densities $r_s = 2$–6 is not exactly known, where k and ω are the wave vector and frequency, respectively. Our knowledge is very approximate [1], and still beset with controversies. We present here an asymptotically exact solution of $S(k,\omega)$ at $T=0$, valid at one particular metallic density $r_s \approx 3.5$, obtained by the recurrence relations method, which may help address some of the issues in this subject.

The dynamics of an electron gas has been most often studied via the frequency moments $c_n(k)$, which are related to $S(k,\omega)$ through the frequency-moment sum rules

$$\tfrac{1}{2} c_n(k) = \int_0^\infty S(k,\omega)\omega^{2n-1} d\omega, \quad n = 0,1,2,\ldots, \tag{1}$$

at $T=0$ [1]. The moments of the density response function are calculable from

$$c_n(k) = (L^n \rho_k, L^n \rho_k), \tag{2}$$

where $L\rho_k = [H,\rho_k]$, H is the Hamiltonian, ρ_k is the density operator, and the inner product means the Kubo scalar product. With $c_n(k)$ one can construct $S(k,\omega)$ uniquely by means of the recurrence relation method [2(a)]. The density relaxation function $\Xi_k(t) = (\rho_k(t), \rho_k)/(\rho_k,\rho_k)$, where t is the time [2(b)], is connected to $S(k,\omega)$ as follows:

$$\tilde{S}(k,\omega) \equiv S(k,\omega)/c_0(k) = -\pi^{-1} \mathrm{Im}[1 - z\hat{\Xi}_k(z)]_{z=i\omega+\epsilon}, \tag{3}$$

where $\hat{\Xi}_k(z) = \mathcal{L}\Xi_k(t)$, and $\mathcal{L}$ is the Laplace transform operator. Now generally

$$\hat{\Xi}(z) = 1/z + \Delta_1/z + \Delta_2/z + \cdots \text{ (continued fraction)}, \tag{4}$$

where each Δ_n can be expressed entirely in terms of the ratios $\lambda_{n-1},\ldots,\lambda_0$, where $\lambda_n = c_{n+1}/c_n$ [3]. Hence, $S(k,\omega)$ may be obtained, given $\{c_n\}$ or $\{\lambda_n\}$ independently.

We consider the standard homogeneous 3D electron gas model defined by $H = H_0 + V$, where H_0 is the kinetic energy (KE) and V is the Coulomb interaction energy with the potential $v(r) = e^2/r$ [1]. The moments for this model can be thus calculated by (2). For $k \gg k_F$ (k_F the Fermi wave vector), we find that ratios of the successive moments can be given as

$$\lambda_n \equiv c_{n+1}/c_n = P + nQ + \sum_{i=1}^{n} R_i + o(k^{-2}), \quad n = 0,1,2,\ldots, \tag{5}$$

$$P = k^4 - (4x/3)k^2 + \tfrac{16}{9}x^2 - \tfrac{16}{5}y + \tfrac{1}{3}\omega_p^2[1 + 2g(0)], \tag{5a}$$

$$Q = (16x/3)k^2 - \tfrac{16}{9}x^2 + \tfrac{16}{5}y, \tag{5b}$$

$$R_n = -2^6/3(n-1)(2n-3)A - 2^7/9(n-1)B, \tag{5c}$$

$$A = x^2 - \tfrac{3}{5}y, \tag{6a}$$

$$B = x^2 - \tfrac{3}{16}\omega_p^2[1 - g(0)], \tag{6b}$$

where k is now expressed in units of k_F, $\hbar = 1$, ω_p is the plasma frequency expressed in units of ϵ_F, the Fermi energy, and $g(0)$ is the pair correlation function at the origin; x and y are the average one-particle KE and KE squared, expressed in units of ϵ_F and ϵ_F^2, respectively [4]. Evidently λ_n [(5)] is r_s dependent through x, y, $g(0)$, and ω_p.

If λ_n were independent of n, e.g., $\lambda_n = \lambda$, (5) would be in the form of a 1D transfer matrix equation, $c_{n+1} = \lambda c_n$, in which λ would act as an eigenvalue. But it is not; λ_n is nonlinearly dependent on n through R_n. Hence, a general solution even for large k is probably precluded. To obtain a particular solution, we make the following assumption (to be justified): At $r_s = r_s^*$, $A = B = 0$. Then, to order k^0, (5) under the assumption becomes

$$\lambda_n(r_s = r_s^*) \equiv \lambda_n^* = P^* + nQ^* = (n+s)Q^*, \quad s \equiv P^*/Q^*, \tag{7}$$

where an asterisk on a real quantity means that its density is set at $r_s = r_s^*$. Then, valid to this order of k, $\lambda_n^* - \lambda_{n-1}^* = Q^*$, i.e., the difference is now independent of n.

Since Δ_n is a function of $\lambda_{n-1}, \ldots, \lambda_0$ [5], (7) implies that $\{\Delta_n^*\}$ is composed of two families:

$$\Delta_{2n-1}^*(k) = (n-1+s)Q^*, \tag{8a}$$

$$\Delta_{2n}^*(k) = nQ^*, \tag{8b}$$

$n = 1,2,\ldots$. Substituting (8a) and (8b) in (4), we obtain

$$\hat{\Xi}_k(z) = \frac{z}{Q^*\Gamma(s)} \int_0^\infty \frac{e^{-u}u^{s-1}\,du}{u + z^2/Q^*} \tag{9}$$

if $\mathrm{Re}\, s > 0$ and $z \neq \pm i|\xi|$ [6]. Finally substituting (9) in (3), we obtain

$$\tilde{S}^*(k,\omega) = [\omega^{2s}/Q^{*s}\Gamma(s)]e^{-\omega^2/Q^*}, \tag{10}$$

where the frequency ω is in units of ϵ_F. Thus, (10) is an asymptotically exact expression for the dynamic structure factor of the electron gas at $r_s = r_s^*$ *subject to our assumption.* Observe that $\tilde{S}^*(k,\omega)$ is smoothly peaked at $\omega = \bar{\omega}$, i.e., $(\partial/\partial\omega)S^*(k,\bar{\omega}) = 0$, $\bar{\omega} = (sQ^*)^{1/2}$, which may be interpreted as the recoil frequency (since, e.g., $\bar{\omega} \to \hbar k^2/2m$ as $k \to \infty$).

We shall now turn to justify our assumption $A^* = B^* = 0$. It asserts that there exist unique relationships between x, y, and $g(0)$ at $r_s = r_s^*$. These relationships cannot be determined by the frequency moment sum rules (1). But if they exist, one may be able to deduce them from other general properties of the dynamic structure factor. If, for example, $\mathcal{T}$ denotes the one-particle KE in 3D, its average value at $T = 0$ is given as follows:

$$\langle \mathcal{T}^n \rangle = \lim_{k\to\infty} \frac{2n+1}{(4\omega_r)^n} \int_0^\infty S(k,\omega)(\omega - \omega_r)^{2n}\,d\omega, \tag{11}$$

$$n = 1,2,\ldots,$$

where ω_r is the recoil frequency [7]. Recall that $\langle \mathcal{T} \rangle = x$ and $\langle \mathcal{T}^2 \rangle = y$, where x and y are parameters of the moments. See (5a)-(5c). Since $S(k,\omega)$ is valid for large k, it may be used in (11) to calculate $\langle \mathcal{T}^n \rangle$ at $r_s = r_s^*$. Substituting (10) in (11), with $\omega_r = \omega_r^* = \bar{\omega}$, we obtain, when $n = 1$ and 2,

$$\langle \mathcal{T} \rangle_{r_s^*} = x^*, \tag{12a}$$

$$\langle \mathcal{T}^2 \rangle_{r_s^*} = \tfrac{5}{3} x^{*2} = y^*. \tag{12b}$$

(12a) indicates that the average KE is given correctly by (10). It is a necessary condition for the validity of our expression for $\tilde{S}^*(k,\omega)$, here obtained independently of the frequency moment sum rules (1). Equation (12b) indicates that $A^* = x^{*2} - \frac{3}{5} y^* = 0$, i.e., the first part of the assumption is satisfied.

There is a relation due to Kimball [8], which relates $g(0)$ to the large-k form of the static structure factor $S(k)$ if $r_s \neq 0$, given as follows:

$$\mu \equiv \lim_{k\to\infty} \{k^4[1 - S(k)]\} = \tfrac{1}{2}\omega_p^2 g(0). \tag{13}$$

Since $S(k)$ may be obtained from $S(k,\omega)$ by $S(k) = \rho^{-1}\int_0^\infty d\omega\, S(k,\omega)$, where ρ is the number density, (13) can be used to establish a relationship between $g(0)$ and x or y. Using (10), we obtain $S^*(k)$ via the structure-factor sum rule,

$$S^*(k) = k^2 Q^{*-1/2}\Gamma(s+1/2)/\Gamma(s+1) = 1 - \{\tfrac{10}{9} x^{*2} - \tfrac{6}{5} y^* + \tfrac{1}{6}\omega_p^{*2}[1 + 2g^*(0)]\}k^{-4} + o(k^{-6}). \tag{14a}$$

Now $\mu^* = \frac{1}{2}\omega_p^{*2} g^*(0)$ from (13) by setting $r_s = r_s^*$. Identifying μ^* from (14a), i.e., the coefficient of k^{-4} therein [9], we obtain (without using $A^* = 0$) the desired relationship:

$$\tfrac{1}{6}\omega_p^{*2}[1 - g^*(0)] = -\tfrac{10}{9} x^{*2} + \tfrac{6}{5} y^*. \tag{14b}$$

Hence, by (14b),

$$B^* = x^{*2} - \tfrac{3}{16}\omega_p^{*2}[1 - g^*(0)] = \tfrac{9}{4} A^*. \tag{14c}$$

Since $A^* = 0$ by (12b), $B^* = 0$ also by (14c). It shows that A and B vanish simultaneously at one unique value of r_s. Therefore, we conclude that (10) is an asymptotically exact solution of the dynamic structure factor at $r_s = r_s^*$.

The possible usefulness of our asymptotic expression (10) evidently rests on the value of r_s^*. Since the one- and two-body distribution functions are not analytically known, we are unable to determine it exactly. But we can attempt to obtain it approximately by numerical means. To do so, it is necessary to know the values of x, y, and $g(0)$ for a range of r_s. Several people have calculated $g(0) \approx 0.3$-0.01 for $r_s = 1$-10. Although different methods yield somewhat different values, most seem to agree to the two significant places. The values given by, for example, Lantto *et al.* [10], and Utsumi and Ichimaru [10] are remarkably consistent in spite of different methods used. Several people [10,11] have also calculated x for $r_s = 1$-10. Their values differ at most by about 4%. To our knowledge, there are no published calculations of y. Lantto [11] calculated x by using the momentum distribution $n(k)$ obtained by a Jastrow variational method. He similarly calculated y, which, being more sensitive to the tail of $n(k)$, is probably somewhat less accurate than x. We use Lantto's x and y, also Lantto *et al.*'s $g(0)$, all obtained by the *same* variational method. (For a consistent determination, they must all be obtained by one method.) Shown in Fig. 1 is A and B vs r_s, where we observe that A and B vanish simultaneously at $r_s = r_s^* = 3.5$. Allowing for different methods, we conclude that $r_s^* = 3.5 \pm 0.2$, and hence also $\omega_p^* = 1.76 \pm 0.10$.

The fact that r_s^* falls within the metallic density range

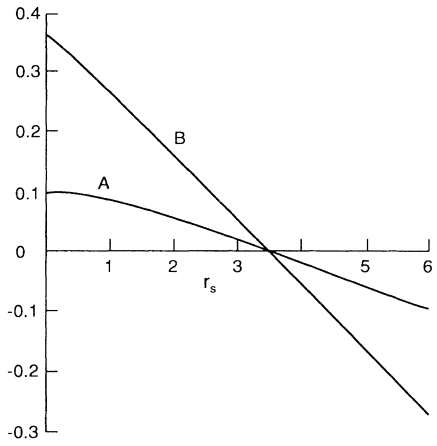

FIG. 1. A and B vs r_s. See Eqs. (6a) and (6b).

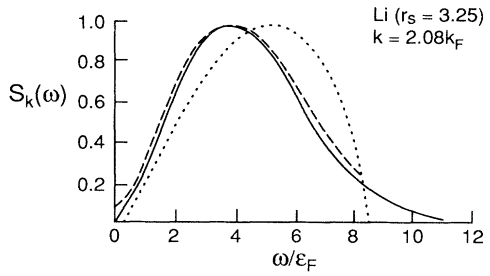

FIG. 2. $S(k,\omega)$ vs ω. Experimental (dashed line), Ref. [12(a)]; Eq. (10) (solid line); RPA (dotted line). The vertical scale is arbitrary.

makes our asymptotic solution (10) meaningful. The value of r_s^* is in fact close to that of Li ($r_s=3.25$). Fortunately there is an old measurement of $S(k,\omega)$ for Li at $k=2.08k_F$ [12(a)]. This value of k is probably large enough to permit a comparison of the measurement with our asymptotic result. Shown in Fig. 2 is the measured dynamic structure factor for Li against the theoretical one (10) with k set at the experimental value. The position of the maximum $S(k,\omega)$ is nearly indistinguishable [12(b)]. Overall the agreement appears good. Also shown is the RPA result at the same value of k, which is markedly different as is well known by now [13].

We shall now discuss the significance of our result: (i) $A^*=B^*=0$, which we have justified above, consists of two exact physical relations at $r_s=r_s^*$: $y=\frac{5}{3}x^2$, $g(0)=1-\frac{16}{3}(x/\omega_p)^2$. Both imply that the momentum distribution $n(k)$ is far from that of the ideal ($r_s=0$). Although having arisen in a high-k analysis of the moments, these relations do not refer to k. Thus, they may be used, for example, as a test of accuracy for numerical methods of calculating the one- and two-body distribution functions. (ii) At $r_s\approx 3.5$, $g(0)\approx 0.08$. An electron has a very small but finite probability of being at another's center. [At this density, $g^{\mathrm{RPA}}(0)<0$.] The physical requirement of a non-negative $g(0)$ means that $\mu\geq 0$ [see (13)]. In our work, $\mu^*\approx 0.13$ [see (14a)]. At high k, x is an essential parameter in the moments, hence, also in $S(k)$ and $S(k,\omega)$. The value of x is strongly r_s dependent, e.g., $x^*\approx 0.73$ versus $x(r_s=0)=0.6$. (iii) $\tilde{S}^*(k,\omega)$ is of a quadratic maximum, centered on $\omega=\bar{\omega}=\hbar k^2/2m-\frac{2}{3}x^*+\cdots$ (natural units), and it has high- and low-frequency tails. These features recall the work of Sokol *et al.* [7] on the inelastic scattering of neutrons from liquid ^{3}He in the "impulsive" domain ($k\gg 2k_F$), where only single-particle scattering is said to occur. Our structure factor at $k\sim 2k_F$ (see Fig. 2) also has an appearance of scattering from a system in single-particle states. But they are not the free particle states because, at this k, the recoil frequency is still not that of a free particle. (iv) As k becomes larger, the assumption becomes less important to the moments. Thus, in the "impulsive" domain, (10) can be essentially free of the constraint $r_s=r_s^*$ and be applicable at $r_s\neq r_s^*$. If k is not very large ($k\sim 2k_F$), in the neighborhood of $r_s=r_s^*$ one may obtain $\tilde{S}(k,\omega)$ approximately by our perturbation method using (10) as a basis [14]. (v) The structure of the moments (7) is also realizable in other systems, e.g., liquid ^{3}He, a semiclassical gas [15], and magnetic solids [16]. Thus (10) has other possible applications [17].

Finally the relaxation function $\Xi_k(t)$ can be obtained from (9):

$$\Xi_k(t)=\mathcal{L}^{-1}\hat{\Xi}_k(z)$$
$$=\frac{1}{\Gamma(s)}\int_0^\infty e^{-u}u^{s-1}\cos(Q^*t^2u)^{1/2}du$$
$$=\Phi(s,\tfrac{1}{2};-Q^*t^2/4), \qquad (15)$$

where Φ is the Kummer function [18]. Observe that $\Xi_k(-t)=\Xi_k(t)$ and $\dot{\Xi}_k(t=0)=0$ as required [2(a)]. The short-time behavior is elementary. The long-time behavior is given by an asymptotic property of the Kummer function [19],

$$\Xi_k(t\to\infty)=\Gamma(\tfrac{1}{2})/\Gamma(\tfrac{1}{2}-s)(Q^*t^2/4)^{-s}$$
$$\sim t^{-2s}\quad (s\neq\tfrac{1}{2}), \qquad (16)$$

another example of slow decay in a Hermitian system [20]. Observe, however, that the exponent $2s\simeq 3k^2/8x^*$ is already far from the classical value $\frac{3}{2}$ when $k=2k_F$.

The work has been supported by the NSF, ARO/CRDEC, and the University of Georgia Office of the Vice President for Research; also by KOSEF, SNU-CTP, and the Basic Science Research Institute Program of the Ministry of Education of Korea.

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and Phys. Rev. Lett. **49**, 1072 (1982). (b) We adopt the common notation of linear response theory. In the recurrence relations notation, $\Xi_k(t)=a_0(t)$.

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