Off-diagonal long-range order, pair distribution function, and structure factor of the ideal Fermi gas in D dimensions and Price's inequality

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(Received 29 June 1994)

The one-particle density matrix in the coordinate representation is calculated for the ideal Fermi gas in general D dimensions and a slow decay form of off-diagonal long-range order (ODLRO) is demonstrated therein. The pair distribution function and the structure factor are deduced from the one-particle density matrix. Their deviations from the classical values are viewed as a measure of the quantum phase, manifesting the existence of ODLRO. An upper bound on the structure factor due to Price [Phys. Rev. **94**, 257 (1954)] is tested with our general solution and is also applied to the interacting electron gas.

PACS number(s): 05.30.Fk

I. INTRODUCTION

Some years ago, in an illuminating paper, Luban and Revzen showed a new way of viewing the origin of the phase transition in the ideal Bose gas [1]. It is the existence of off-diagonal long-range order (ODLRO) in the one-particle density matrix ρ_1 in the coordinate representation, to which the singular behavior of the thermodynamic functions can be traced. In particular, the onset of this order can account for the divergences of C_P and κ_T at $T=T_c$, where the condensate fraction is still strictly zero and also at $T<T_c$, where the condensed fraction is finite. Luban and Revzen were applying the concept due to Yang [2] to the ideal Bose gas by making several of the thermodynamic functions reveal therein the existence or absence of ODLRO.

Yang's idea was that in quantum many-body systems such as the ideal Bose gas there is a new thermodynamic phase of quantum origin. Thermodynamic functions describing it can be shown to manifest the existence of ODLRO. This order arises from the symmetries of many-body wave functions. Hence, it can quantitatively define a quantum regime. The order, much like other orders, e.g., magnetization, can vanish with thermal fluctuations. Yang's concept has now become an important means with which to study macroscopic properties of quantum origin in many-body systems [3].

If the existence of ODLRO means the appearance of a new thermodynamic phase, microscopic correlation functions like the pair distribution function cannot be impervious to its manifestation. Any change in them in going from the quantum to the classical regime must be attributable to the existence or absence of ODLRO. Indeed the work of Luban and Revzen suggests as much. They show for the ideal Bose gas that the one-particle density matrix entirely determines the behavior of the pair distribution function and that the large-distance behavior changes strikingly as T crosses T_c. The existence of ODLRO could perhaps be even more effectively observed in the structure factor, which is sensitive to the large-distance behavior in the pair distribution function.

The ideal Fermi gas does not have a phase transition and usually only its ground state is of any interest. One might therefore think that Yang's concept is not useful here. However, the Fermi gas in the ground state behaves nonclassically also because of the symmetry of its wave function. That is, there is a corresponding new phase of quantum origin which we contend implies the existence of some form of ODLRO. This order in a Fermi gas evidently cannot be finite at large distances there being no condensation as in the Bose gas. Nevertheless, in our view, ODLRO can still be said to exist if it vanishes slowly with the distance. It exists if it is manifested in, e.g., the structure factor by being significantly different from its classical value. To describe the fermion thermodynamic phase, we propose to extend Yang's original concept. This extended version is not really novel. Luban and Revzen have already shown that the onset of a phase transition in the Bose gas is signaled by a slow decay of ODLRO.

The ideal Fermi gas has been historically an important model for the conduction electrons in metals. Many of its ground state properties in $D=3$ (D dimensions) are exhaustively described in standard texts, but seldom from the point of view of ODLRO in ρ_1. In these treatments it is customary to obtain, for example, the structure factor $S(k)$ first, where k is the wave vector, and then by a Fourier transform the pair distribution function $g(r)$, where r is the separation distance of a pair of identical particles. Luban and Revzen thus suggest an alternative way of obtaining $g(r)$ first, itself obtained from ρ_1, from which then $S(k)$ afterward. One practical advantage of this approach is that ρ_1 can be obtained in any value of D, hence $g(r)$ and also $S(k)$. An exact knowledge of the structure factor is of general theoretical interest. There is, for example, a bound on the structure factor due to Price [4]. Our D-dimensional solution can provide a rigorous test for the validity of this bound perhaps for the first time. Relevance of studying thermodynamic functions in D dimensions has been addressed elsewhere [5,6].

II. ONE-PARTICLE DENSITY MATRIX

We consider a system of N ideal Fermi particles in a D-dimensional volume V in thermal equilibrium. Following Luban and Revzen we introduce the Fermi version of the one-particle density matrix in the coordinate representation,

$$\rho_1(r,r')=\sum_\sigma \langle \psi_\sigma^\dagger(r)\psi_\sigma(r')\rangle \ , \tag{1}$$

where the angular brackets mean the grand canonical ensemble average. Here $\psi_\sigma(r)$ denotes a spin-σ field operator at position r, satisfying the Fermi commutation relations:

$$[\psi_\sigma(r),\psi_{\sigma'}^\dagger(r')]_+=\delta(r-r')\delta_{\sigma\sigma'} \ , \tag{2a}$$

$$[\psi_\sigma(r),\psi_{\sigma'}(r')]_+=[\psi_\sigma^\dagger(r),\psi_{\sigma'}^\dagger(r')]_+=0 \ . \tag{2b}$$

We shall assume that our system is translationally invariant, e.g., $\rho_1(r,r')=\rho_1(|r-r'|)$. Writing

$$\psi_\sigma(r)=V^{-1/2}\sum_k e^{ik\cdot r}a_{k\sigma} \ ,$$

etc., we can express (1) as

$$\tilde\rho_1(r)\equiv\rho_1(r)/\rho=N^{-1}\sum_{k\sigma}\langle \hat n_{k\sigma}\rangle e^{ik\cdot r} \ , \tag{3}$$

where $\rho=N/V$ and $\hat n_{k\sigma}=a_{k\sigma}^\dagger a_{k\sigma}$ the number operator. Except for the spin sum, the one-particle density matrix (3) has the same form as that for the ideal Bose particles.

When $T=0$, $\langle \hat n_{k\sigma}\rangle=\theta(k_F-|\mathbf{k}|)$, a step function, where k_F is the Fermi wave vector. One can evaluate (3) in the ground state as follows [6]. If $D\geq 3$,

$$\begin{aligned}\tilde\rho_1(r)&=\left[\frac{2}{(2\pi)^D\rho}\right]\left[\frac{2\pi^{(D-1)/2}}{\Gamma((D-1)/2)}\right]\int_0^{k_F}k^{D-1}dk\int_0^\pi \sin^{D-2}\theta e^{ikr\cos\theta}d\theta\\ &=\frac{2\Gamma(D/2+1)}{\sqrt{\pi}\Gamma((D-1)/2)}\int_0^1 k^{D-1}dk\int_0^\pi \sin^{D-2}\theta e^{ikx\cos\theta}d\theta \ ,\end{aligned} \tag{4}$$

where Γ is the gamma function, $x=rk_F$. We have used $k_F^D/\rho=2^{D-1}\pi^{D/2}\Gamma(D/2+1)$. The second double integral, which we shall denote as $I_{D/2}(x)$, is now dimensionless.

Using the integral representation of the Bessel function

$$J_\nu(z)=\frac{(z/2)^\nu}{\sqrt{\pi}\Gamma(\nu+\frac12)}\int_0^\pi \sin^{2\nu}\theta\cos(z\cos\theta)d\theta \ , \tag{5}$$

we can express $I_{D/2}(x)$ as follows. Writing $m=D/2$,

$$I_m(x)=\sqrt{\pi}\,\Gamma(m-\tfrac12)(2/x)^{m-1}\int_0^1 k^m J_{m-1}(kx)dk=\sqrt{\pi}\,2^{m-1}\Gamma(m-\tfrac12)x^{-m}J_m(x) \ , \tag{6}$$

where we have used the relation $\int_0^z t^\nu J_{\nu-1}(t)dt=z^\nu J_\nu(z)$. Hence, together

$$\tilde\rho_1(r)=2^m\Gamma(m+1)x^{-m}J_m(x) \ , \quad m=0,1/2,1,3/2,\ldots \tag{7a}$$

$$=\pi^{-1/2}2^{m+1/2}\Gamma(m+1)x^{-m+1/2}j_{m-1/2}(x) \ , \quad m=1/2,3/2,\ldots \ , \tag{7b}$$

where $x=rk_F$.

We note that although our original expression (4) is valid if $D\geq 3$, our final result (7a) is valid for any nonnegative values of D by virtue of analytic continuation. In Table I we have listed $\tilde\rho_1(r)$ in several low dimensions. Evidently there are two families, D even and D odd. When $r\to\infty$, the nonoscillatory part of the density matrix vanishes as $r^{-D/2-1/2}$. This is a slow decay [7], which according to our view, implies the existence of ODLRO in $\rho_1(r)$. We shall see that the pair distribution function and the structure factor for the ideal Fermi gas in the ground state, in particular their deviations from the classical values, result entirely from this density matrix just as Luban and Revzen have shown for the ideal Bose gas.

TABLE I. Normalized one-particle density matrix in D dimensions. $x=rk_F$.

D	$\tilde\rho_1(x)$	D	$\tilde\rho_1(x)$
0	$J_0(x)$	1	$j_0(x)$
2	$2x^{-1}J_1(x)$	3	$3x^{-1}j_1(x)$
4	$8x^{-2}J_2(x)$	5	$15x^{-2}j_2(x)$

III. PAIR DISTRIBUTION FUNCTION

The pair distribution function $g(rr')$, a two-particle density matrix in the coordinate representation, has the following standard definition:

$$\begin{aligned}g(r,r')&=\rho^{-2}\sum_{\sigma\sigma'}\langle \psi_\sigma^\dagger(r)\psi_{\sigma'}^\dagger(r')\psi_{\sigma'}(r')\psi_\sigma(r)\rangle &(8a)\\ &=N^{-2}\sum_{\sigma\sigma'}\sum_{pqk}\langle a_{p\sigma}^\dagger a_{q\sigma'}^\dagger a_{q-k\sigma'}a_{p+k\sigma}\rangle e^{ik\cdot(r-r')} \ . &(8b)\end{aligned}$$

It is defined so that $g(|r-r'|\to\infty)=1$ in this translationally invariant system.

For the ideal Fermi gas, just as for the ideal Bose gas, nonzero contributions to the sum in (8b) arise only if $\mathbf{k}=0$ and $\mathbf{k}=\mathbf{p}-\mathbf{q}\neq 0$. Note that $\langle \hat{n}_{p\sigma}\hat{n}_{q\sigma'}\rangle = \langle \hat{n}_{p\sigma}\rangle\langle \hat{n}_{q\sigma'}\rangle$ if $\mathbf{p}\neq\mathbf{q}$ or $\sigma\neq\sigma'$ and also $\langle \hat{n}_{p\sigma}\rangle=\langle \hat{n}_{p\sigma'}\rangle$. Using the above properties one an show that

$$g(r)=1-\tfrac{1}{2}[\tilde{\rho}_1(r)]^2 \tag{9}$$

which is valid at any temperature and in any D [8]. This simple relation (9) is useful. For example, $g(r=0)=\frac{1}{2}$, a well-known result. Also it gives an upper bound on $g(r)$: $g(r)\le 1$. Equation (9) may be compared with say, $g^B(r)$, the pair distribution function for the ideal Bose gas at $T>T_c$ given by Luban and Revzen

$$g^B(r)=1+[\tilde{\rho}_1^B(r)]^2 \ , \tag{10}$$

which gives a lower bond $g^B(r)\ge 1$ [9(a)] and also $g^B(r=0)=2$, somewhat less well known [9(b)].

The inequalities, $g^F(r)\le 1$ and $g^B(r)\ge 1$, for the ideal Fermi and Bose gases, respectively, are interesting. First of all, in the *classical* limit, statistics cannot play any role, i.e., $g^F(r)=g^B(r)=g^C(r)=1$, where $g^C(r)$ refers to the classical ideal gas. Thus, $\tilde{\rho}_1(r)$ must vanish in the classical limit as one can readily show [10]. The departure from the classical value is sometimes attributed to the existence of a quasiforce, which acts repulsive for Fermi particles and attractive for Bose particles [11]. In actual fact, it is the existence of ODLRO in the one-particle density matrix to which any departure from the classical behavior must be attributed.

Using (7a) in (9), the pair distribution function in D at $T=0$ is explicitly

$$g(r)=1-\tfrac{1}{2}[cx^{-m}J_m(x)]^2 \ , \tag{11}$$

where $m=D/2$, $x=rk_F$, and $c=2^m\Gamma(m+1)$. We shall note a few elementary properties of $g(r)$ in D:

i. $g(r\to 0)=\dfrac{1}{2}+\dfrac{x^2}{2(D+2)}+0(x^4)$.

ii. $\partial g(r)/\partial r=ax^{-2m}J_m(x)J_{m+1}(x)$, $a\equiv c^2k_F$. Hence, $\partial g(r\to 0)/\partial r=k_F r/(D+2)$, which also follows from (i).

iii. Since the Bessel functions are bounded, i.e., $|J_m(x)|\le 1$ if $m\ge 0, g(r\to\infty)=1$.

iv. The asymptotic behavior of $g(r)$ is

$$g(r\to\infty)-1=-\pi^{-1}c^2x^{-D-1}\cos^2[x-\pi(D+1)/4] \ .$$

v. $\frac{1}{2}\le g(r)\le 1$.

IV. STRUCTURE FACTOR IN D DIMENSIONS

The structure factor for the ideal Fermi gas at $T=0$ is known in $D=1$–3, usually obtained by $S(k)=N^{-1}\sum_{p\sigma}$, with the restriction $|\mathbf{p}|<k_F$ and $|\mathbf{p}+\mathbf{k}|>k_F$ [12]. If $|\mathbf{k}|<2k_F$, $S(k)$ is the volume of the Fermi sphere, symmetrically cut off at the top and the bottom to the depth $k/2$ from the center of its sphere. A dependence on k and D results from the cutoff. If $|\mathbf{k}|>2k_F$, it is that of the full uncut Fermi sphere, losing the k and D dependence as a result. A similar loss of the k and D dependence takes place if $S(k)$ is imposed the classical limit [13]. The coordinate space origin of this discontinuity at $2k_F$ is curious since the pair distribution function is a completely smooth function of the separation distance. Evidently it stems from oscillations of the Bessel function.

The structure factor $S(k)$ is related to the pair distribution function $g(r)$, hence, to $p_1(r)$, through the well-known formula: If $\mathbf{k}\neq 0$,

$$S(k)-1=\rho\int d^Dr\, e^{-i\mathbf{k}\cdot\mathbf{r}}[g(r)-1] \tag{12a}$$

$$=-\rho/2\int d^Dr\, e^{-i\mathbf{k}\cdot\mathbf{r}}[\tilde{\rho}_1(r)]^2 \ . \tag{12b}$$

Substituting (7a) for $\tilde{\rho}_1(r)$ in (12b) we obtain

$$S(k)-1=-\frac{2\Gamma(m+1)}{\sqrt{\pi}\Gamma(m-1/2)}\int_0^\infty dx\, x^{-1}J_m^2(x)\int_0^\pi d\theta \sin^{2m-2}\theta\cos(kx\cos\theta) \ , \tag{13}$$

where k now is in units of k_F. Using (5) we can reduce (13) to

$$=-\frac{2^m\Gamma(m+1)}{k^{m-1}}\int_0^\infty x^{-m}J_m^2(x)J_{m-1}(x)dx \ . \tag{14}$$

The integral may be evaluated by first reducing the squared Bessel function by means of Neumann's integral [14]:

$$J_\nu^2(z)=\frac{1}{\pi}\int_0^\pi J_{2\nu}(2z\cos\psi)d\psi \ . \tag{15}$$

Thus,

$$Q\equiv\int_0^\infty x^{-m}J_m^2(x)J_{m-1}(kx)dx$$
$$=\frac{1}{\pi}\int_0^\pi P_m(\psi)d\psi \ , \tag{16}$$

where

$$P_m(\psi)=\int_0^\infty x^{-m}J_{m-1}(kx)J_{2m}(2x\cos\psi)dx \ . \tag{17}$$

Equation (17) is the form of a discontinuous Bessel integral: For $\nu>\mu>-1$,

$$\int_0^\infty x^{\mu-\nu+1}J_\mu(ax)J_\nu(bx)dx=\begin{cases}0 \quad \text{if } |a|>|b|,\\ \dfrac{2^{\mu-\nu+1}a^\mu(b^2-a^2)^{\nu-\mu-1}}{b^\nu\Gamma(\nu-\mu)} \quad \text{if } |b|>|a| \ .\end{cases} \tag{18}$$

Hence, we choose $a=k/2\equiv q$, $b=\cos\psi$, $\mu=m-1$, $\nu=2m$. Then, $\mu-\nu+1=-m$ and the condition $\nu>\mu>-1$ is satisfied if $m>0$ (although $m=0$ may also be satisfied by analytic continuation). Using the above stated choice we can now evaluate (17): (i) If $q>1$ (i.e., $k>2k_F$), then $q>|\cos\psi|$ for $\psi=(0,\pi)$ and $P_m(\psi)=0$ for $m>0$. Hence, $S(q)=1$. (ii) if $q<1$, $q<|\cos\psi|$ for the intervals $\psi=(0,\psi_1)$ and (ψ_2,π), where $\psi_2=\pi-\psi_1$ and $\psi_1=\cos^{-1}q$. Hence, if $q<1$ (i.e., $k<2k_F$),

$$Q=-\frac{q^{m-1}}{\pi\Gamma(m+1)}\int_0^{\psi_1}(1-q^2/\cos^2\psi)^m d\psi \tag{19}$$

and

$$S(q)-1=-\frac{2}{\pi}\int_0^{\psi_1}(1-q^2/\cos^2\psi)^m d\psi \; . \tag{20}$$

The RHS of (20) is in the form of an integral representation of the hypergeometric function (hgf) [15]: If $c>b>0$,

$$F(abcz)=\frac{\Gamma(c)}{\Gamma(b)\Gamma(c-b)}\int_0^1 t^{b-1}(1-t)^{c-b-1}(1-zt)^{-a}dt \; . \tag{21}$$

For (20) the condition $c>b>0$ is equivalent to $m>0$. Hence, for $q<1$, where again $q=k/2k_F$,

$$S(q)=1-[\Gamma(m+1)/\sqrt{\pi}\Gamma(m+3/2)](1-q^2)^{m+1/2}F(m+1/2,1/2,m+3/2,1-q^2) \; . \tag{22}$$

The above result is useful for studying the behavior of $S(q)$ near $q=1$, but not near $q=0$.

To obtain such an expression we consider the following linear transformation of the hgf [15]: If $c-a-b\neq$ negative integers,

$$F(abcz)=[\Gamma(c)\Gamma(c-a-b)/\Gamma(c-a)\Gamma(c-b)]F(a,b,a+b-c+1,1-z)$$
$$+[\Gamma(c)\Gamma(a+b-c)/\Gamma(a)\Gamma(b)](1-z)^{c-a-b}F(c-a,c-a-b+1,1-z) \; . \tag{23}$$

For the parameters of the hgf of (22), $c-a-b=\frac{1}{2}$. Hence,

$$S(q)=[2\Gamma(m+1)/\sqrt{\pi}\,\Gamma(m+1/2)]q(1-q^2)^{m+1/2}F(m+1,1,3/2,q^2) \; . \tag{24}$$

The above still contains $(1-q^2)$. To remove it we introduce one more transformation, this one due to Euler [15]: If $c\neq$ negative integers and $|z|<1$,

$$F(abcz)=(1-z)^{c-a-b}F(c-a,c-b,c,z) \; . \tag{25}$$

Identifying $a=\frac{1}{2}$, $b=\frac{1}{2}-m$, $c=\frac{3}{2}$ we obtain finally that for $q<1$

$$S(q)=[2\Gamma(m+1)/\sqrt{\pi}\Gamma(m+1/2)]qF(1/2-m,1/2,3/2,q^2)=qF(\tfrac{1}{2}-m,\tfrac{1}{2},\tfrac{3}{2},q^2)/F(\tfrac{1}{2}-m,\tfrac{1}{2},\tfrac{3}{2},1) \; . \tag{26}$$

Observe that m appears in but one parameter of the hgf of (26). It makes it simple to deduce a dimensional relationship. Also, if $m=D/2$ is a half integer (D odd), the hgf is a polynomial in q^2. If m is an integer (D even), it is a function of q^2 [16].

V. BEHAVIOR OF STRUCTURE FACTOR

We shall now show a few general features of the structure factor $S_m(q)$ as a function of both $q=k/2k_F$ and $m=D/2$. For a fixed m, the behavior near $q=0$ and 1 is interesting. For $q\rightarrow 0$, the useful form is (26), which we write as

$$S_m(q)=2\pi^{-1}\Omega_m qF(\tfrac{1}{2}-m,\tfrac{1}{2},\tfrac{3}{2},q^2) \; , \tag{27}$$

where

$$\Omega_m=\Gamma(\tfrac{1}{2})\Gamma(m+1)/\Gamma(m+\tfrac{1}{2}) \tag{28a}$$

$$=[m/(m-\tfrac{1}{2})]\Omega_{m-1} \; , \quad m\neq\tfrac{1}{2} \; . \tag{28b}$$

We list a few Ω_m's: $\Omega_0=1$, $\Omega_1=2$, $\Omega_2=\frac{8}{3}$; $\Omega_{1/2}=\pi/2$, $\Omega_{3/2}=3\pi/4$, $\Omega_{5/2}=15\pi/16$.

For $q\rightarrow 0$ one may replace the hgf in (27) by unity to order $o(q^2)$. Hence, immediately,

$$S_m(q\rightarrow 0)=2\pi^{-1}\Omega_m q \; . \tag{29}$$

Thus, $S_m(q)$ is linear in q near the origin and the slope is positive, depending on D. This is very different from the behavior in the ideal Bose gas [17].

To study the behavior near $q=1$ we turn to (22), which to the leading order can be written as

$$S_m(q\rightarrow 1)=1-\pi^{-1}(m+\tfrac{1}{2})^{-1}\Omega_m(1-q^2)^{m+1/2} \; . \tag{30}$$

Hence,

$$\partial S_m(q\rightarrow 1)/\partial q=2\pi^{-1}\Omega_m(1-q^2)^{m-1/2}$$
$$=\begin{cases}2\pi^{-1}(1-q^2)^{-1/2} \; , & m=0 \; , \\ 1 \; , & m=\frac{1}{2} \; , \\ 0 \; , & m>\frac{1}{2} \; .\end{cases} \tag{31}$$

Since $S_m(q\rightarrow 0)=0$ and $S_m(q\rightarrow 1)=1$, and also, if $m>0$, the derivatives are finite positive and continuous on the interval of q, we can state the bounds: $0<S_m(q)<1$ on $q=(0,1)$. In Appendix A our solution for $S_m(q)$ is further compared with an upper bound given by Price [4].

Next, for a fixed q, we look for a recurrence relation in m for $S_m(q)$ by considering (27). The prefactor Ω_m is simply related to Ω_{m-1} [see (28b)]. Also the hgf in (27) has a very simple contiguous relation because of the values of two of its parameters (differing by one) [15]. An applicable contiguous relation for $F(abcz)$ is

$$(b-a)F(abcz)=-aF(a+1bcz)+bF(ab+1cz)\ , \qquad (32)$$

where $F(ab+1cz)=(1-z)^{-a}$ if $b+1=c$. Turning to (27), let $F_m=F(\frac{1}{2}-m,\frac{1}{2},\frac{3}{2},q^2)$. If the parameters of the hgf in (27) are applied to the above contiguous relation we obtain

$$mF_m=(m-\tfrac{1}{2})F_{m-1}+\tfrac{1}{2}(1-q^2)^{m-1/2}\ . \qquad (33)$$

Hence, for $m\geq 1$,

$$S_m(q)=2\pi^{-1}\Omega_m qF_m$$
$$=S_{m-1}(q)+\pi^{-1}m^{-1}\Omega_m q(1-q^2)^{m-1/2}\ ,$$
$$0<q<1\ . \qquad (34)$$

The second term on the RHS of (34) is a polynomial if m is a half integer. It is of a square root if m is an integer.

According to (34), it is a relationship between m and $m-1$. That is, the relationship is between even-numbered dimensions or odd-numbered dimensions, never between even and odd numbered dimensions, sometimes known as an even-odd effect. One can trace the origin of this even-odd effect observed here to the D-dimensional volume integration, which has a given $D/2$, not D, as its natural parameter. The even-odd effect is manifested in $S_m(q)$ through two independent "seeds:" $S_0(q)=2\pi^{-1}qF(\frac{1}{2},\frac{1}{2},\frac{3}{2}\ q^2)=2\pi^{-1}\sin^{-1}q$ and $S_{1/2}(q)=q$ for D's even and odd, respectively. Using these two seeds as boundary values, we can generate $S_m(q)$ for any value of D. A few of them are listed in Table II. Finally, there is a simple inequality, $S_m(q)\geq S_{m-1}(q)$, $0<q<1$, for D's even or odd separately, owing to the fact that he second term on the RHS of (34) is non-negative.

VI. CONCLUDING REMARKS

The effect of our form of ODLRO is particularly easy to see in the ground state of the ideal Fermi gas, for which $g(r)-1$ and $S(k)-1$ are quantitative measures of the quantum phase in the coordinate and momentum spaces, respectively. The relationship between the two measures is not obvious. For example, if $k>2k_F$, there is no effect of ODLRO in the momentum space. Here all the scattering takes place outside the Fermi sphere, "washing out" Fermi statistics. No analogous behavior exists in finite regions of the coordinate space. For the nonideal Fermi gas it has been postulated that $g(r=0)=Ak^4[1-S(k)]$ as $k\to\infty$, where A contains the coupling constant. Here $S(k)-1$ is not simply a measure of quantum phase since $S(k)\neq 1$ if the nonideal gas is classical.

We have shown that for the ideal Fermi gas, $g(r=0)\neq 0$ and $g'(r=0)=0$. [For the nonideal Fermi gas, $g(r=0)$ and $g'(r=0)$ are believed to be a strong function of r_s.] Also, $g(r\to\infty)-1\sim r^{-D-1}$, a nonexponential decay. This asymptotic form of the pair correlation function appears mainly responsible for the linear behavior of $S(k\to 0)$ in k. For $k<2k_F$ we have found that $S(k,D/2)=S(k,(D-2)/2)+B$, where B is a simple function of k and D. Thus, like the susceptibility [6], the structure factor for the ideal Fermi gas is composed of two distinct families, D even and D odd. They never mix. It is also interesting to note that the structure factor can be given as a function of either $(k/2)^2$ or $1-(k/2)^2$, both expressible in integral forms of the hgf.

Evidently the effect of our form of ODLRO is also present in dynamic quantities like the dynamic structure factor $S(k,\omega)$ since the frequency ω can only act to translate the wave vector k [13]. The effect should be seen in these quantities for the nonideal Fermi gas and it should persist in them in low temperatures. An explicit demonstration of ODLRO in these problems recently studied [18–21] would appear to be of interest.

TABLE II. Structure factor in D dimensions. $q=k/2k_F<1$.

D	$S(q)$
0	$2/\pi[\sin^{-1}q]$
2	$2/\pi[\sin^{-1}q+q(1-q^2)^{1/2}]$
4	$2/\pi\{\sin^{-1}q+q(1-q^2)^{1/2}[1+2/3(1-q^2)]\}$
1	q
3	$q[1+1/2(1-q^2)]$
5	$q[1+1/2(1-q^2)+3/8(1-q^2)^2]$

ACKNOWLEDGMENTS

This work was supported in part by NSF and ARO, and also by the Office of the Vice President for Research, University of Georgia. We thank Dr. H. Leschke for drawing our attention to Ref. [17].

APPENDIX A: STRUCTURE FACTOR AND PRICE'S INEQUALITY

Some years ago, Price [4] showed that the structure factor $S(k)$ at $T=0$ is bounded from above as $S(k)\leq S^{ub}(k)$, where $S^{ub}(k\to 0)=k/2mc$, c the speed of sound, m now the mass of the electron, and $\hbar=1$. One can also show that $S^{ub}(k\to\infty)=1$. The upper bound for $k\to 0$ has had some use in assessing the phonon spectrum obtained in approximate theories of Bose fluids [22,23]. To our knowledge, it has otherwise never been rigorously tested in models. Since the bound is based only on certain dynamic sum rules, it is also applicable to the structure factors of Fermi systems. In fact, the structure factor for the D-dimensional electron gas in the ground state obtained here in Sec. IV provides perhaps the simplest possible nontrivial test.

To test the upper bound for $k\to 0$ we first evaluate the speed of sound c for the electron gas in the ground state from the standard relation $mc^2=2\rho\varepsilon'+\rho^2\varepsilon''$, where $\varepsilon'=\partial\varepsilon/\partial\rho$ and $\varepsilon=E_0/N=(1+2/D)^{-1}\varepsilon_F$, E_0 the ground state energy, and ε_F the Fermi energy. Since $\varepsilon'=(2/D)\rho^{-1}\varepsilon$ we deduce that $mc=k_F/\sqrt{D}$. Hence,

$$S^{ub}(k\to 0)=(D/4)^{1/2}\cdot k/k_F\ . \tag{A1}$$

Now from Eq. (29) we have the exact result

$$S(k\to 0) =[\Gamma(D/2+1)/\sqrt{\pi}\,\Gamma(D/2+\tfrac{1}{2})]k/k_F\ , \tag{A2}$$

with which to compare. Therefore, according to Price, the upper bound for $k\to 0$ as applied to the electron gas means

$$2\Gamma(D/2+1)/\sqrt{\pi D}\ \Gamma(D/2+\tfrac{1}{2})\le 1\ . \tag{A3}$$

It does not seem possible to further reduce the LHS of (A3) nor to prove the inequality generally. But it is easy to see it hold D-by-D: If $D=1$, it is an equality. If $D\ge 2$, it gives an inequality correctly. If $D\to\infty$, the LHS of (A3) may be given as

$$\lim_{D\to\infty} 2\Gamma(D/2+1)/\sqrt{\pi D}\ \Gamma(D/2+\tfrac{1}{2})=\sqrt{2/\pi}<1\ . \tag{A4}$$

The upper bound for $k\to\infty$ is trivially satisfied as an equality since $S(k>2k_F)=1$. It is also possible to test the bound for intermediate $k(0<k<2k_F)$ from the general solution [4(b)]

$$S^{ub}(k)=[(k^2/4m\rho)\tilde{\chi}(k)]^{1/2}\ , \tag{A5}$$

where $\tilde{\chi}(k)$ is the reduced susceptibility, i.e., $\tilde{\chi}(k)=\beta\chi(k)/V$, where $\chi(k)=(\rho_k,\rho_k)$ is the Kubo scalar product of the density operator ρ_k, $\beta=1/k_BT$ and V volume. Note that at $T=0$, $\tilde{\chi}(k\to 0)=\partial\rho/\partial\varepsilon_F=D\rho/2\varepsilon_F=\rho/mc^2$. Since the reduced susceptibility for the D-dimensional electron gas in the ground state is known [6], the upper bound (A5) can be stated explicitly. Although to test the bound generally is complicated, it is straightforward to do so D-by-D as before: If, for example, $D=1$, $\tilde{\chi}(k)>\rho/2\varepsilon_F$ for $0<k<2k_F$. Hence, $S(k)=k/2k_F<S^{ub}(k)$ for $0<k<2k_F$, i.e., no longer equal as was when $k\to 0$. If $D=2$, $\tilde{\chi}(k)=\rho/\varepsilon_F$ for $0<k<2k_F$. Hence, $S^{ub}(k)=\sqrt{2}\,q$, where $q=k/2k_F$. One can see that $S(q)=2/\pi[\sin^{-1}q+q(1-q^2)^{1/2}]<\sqrt{2}\,q$ for $0<q<1$. The inequality may be demonstrated similarly in other values of D.

We shall look at the origin of the equality which exists when $k\to 0$ if $D=1$, as well as when $k\to\infty$ in all D's. Price's inequality derives from certain sum rules with respect to the dynamic structure factor $S(k,\omega)$ where ω is the frequency. Evidently an equality is attained because the dynamic structure factor assumes some special form in these domains. The dynamic structure factor in $D=1$ for $k<k_F$ is constant and nonzero only for an interval, whose width vanishes faster than $k\to 0$. Indeed this form gives an equality. When $k\to\infty$, the dynamic structure factor in all D's become sharply peaked about $\omega=k^2/2m$, also giving an equality [4(b)].

Finally, the upper bound for the structure factor of the *interacting* electron gas can also be obtained from (A5). In the long wavelength limit, to first order $\tilde{\chi}(k\to 0)=v_k^{-1}$, where v_k is the Fourier transform of the Coulomb interaction potential. In $D=3$, where $v_k=4\pi e^2/k^2$, we obtain to first order

$$S^{ub}(k\to 0)=k^2/2m\omega_p\ , \tag{A6}$$

where $\omega_p=(4\pi\rho e^2/m)^{1/2}$ is the plasma frequency. Thus, the structure factor can no longer be linear in k as in the ideal gas. In fact, (A6) is the structure factor obtained when the excitations are limited only to long-wavelength plasmons [24]. In $D=2$, where $v_k=2\pi e^2/k^2$ (i.e., log potential), the same upper bound is obtained with $\omega_p=(2\pi\rho e^2/m)^{1/2}$. In the so-called quasi 2D, where $v_k=2\pi e^2/k$, again (A6) is obtained, but now $\omega_p=(2\pi\rho e^2k/m)^{1/2}$, which is k dependent. As in $D=3$, the structure factor contributed by the long-wavelength plasmons alone can attain the upper bound [25], but the single-particle excitations will lower it below the upper bound [26]. When there are only the plasmons, the dynamic structure factor is effectively in the form of a δ function which explains the equality just as when $k\to\infty$.

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[7] The same density matrix for the ideal Bose gas in $D=3$ decays exponentially if $T>T_c$. It is finite if $T\le T_c$. See [1], Eqs. (16) and (20) therein.

[8] A similar form in $D=3$ was earlier given in N.H. March, *The Many-Body Problem in Quantum Mechanics* (Cambridge University Press, Cambridge, England, 1967), pp. 10–12, as an example of the Dirac density matrix.

[9] (a) If $T<T_c$, we believe that Eq. (10) needs to be modified to read $g^B(r)=1+[\tilde{\rho}_1(r)]^2-n_0^2$, where n_0 is the condensate fraction; see H. Hara and T. Morita, Prog. Theor. Phys. Suppl. **44**, 118 (1969). Observe that now $g^B(r\to\infty)=1$ if one uses $\tilde{\rho}_1(r\to\infty)$ given by Luban and Revzen; see [1] [Eq. (20) therein]. Also, one still has the inequality $g^B(r)\ge 1$ since $\tilde{\rho}_1(r)\ge n_0$. (b) The quantity $g(r=0)$ can be interpreted to be the absolute square of the properly normalized wave function for two identical free particles at zero separation distance. For a pair of Bose particles, the symmetrized wave function gives 2. For a pair of Fermi particles, the antisymmetrized wave function gives 0 for the triplet state and 2 for the singlet state, hence, $\frac{1}{2}$ for the average. But classical free particle states are not symmetrized. Hence, one obtains unity for a pair of classical particles; see, e.g., D. Falkoff in *The Many-Body Problem,* edited by C. Fronsdal (Benjamin, New York, 1962). Also see G. D. Mahan, *Many Particle Physics* (Plenum, New York, 1981), pp. 865 and 866.

[10] As may be clear from [1] [see the discussion after Eq. (14)], the classical regime is one in which $r\gg\lambda$ where λ is the

thermal de Broglie wavelength. Hence, it is not possible to take $r \rightarrow 0$ first if λ is held fixed. If $\lambda \rightarrow 0$ first, then $\rho_1(r)=0$.

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[16] The structure factor can also be obtained by the structure factor sum rule $S(k)=\rho^{-1}\int_0^\infty S(k,\omega)d\omega$ if $S(k\omega)$ is known; M. Long (Ph.D. thesis, University of GA, 1994) used $S(k\omega)$ given in M. H. Lee and J. T. Nelson [J. Math. Phys. **31**, 689 (1990)] to obtain the result of Eq. (26).

[17] For the ideal Bose gas in $D=3$ at $0<T<T_c$, $S(k\rightarrow 0)=Ak^{-2}+o(k^2)$, where $A=8\pi n_0\lambda^{-2}$, n_0 the condensate fraction and λ the thermal de Broglie wavelength; also see K. Baerwinkel, Phys. Kondens. Materie (Berlin) **12**, 287 (1971). If $T>T_c$, the behavior is very similar to that of the ideal semiclassical gas; see M. H. Lee and O. I. Sindoni, Phys. Rev. A **46**, 3028 (1992).

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