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#### PHYSICAL REVIEW B

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# Calculation of the Dielectric Function for a Degenerate Electron Gas with Interactions. I. Static Limit\*

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A new procedure for calculating the frequency- and wave-vector-dependent dielectric response function is described. It is based on decoupling and solving the equations of motion for the Green's functions of the charge-density operators by a moment-conserving method which is discussed. By use of this method an expression for the dielectric function in the static limit ( $\omega \rightarrow 0$ ) is obtained; it depends on a function G(k), for which numerical values are calculated and tabulated. Evidence that the procedure described here leads to reliable values of G(k) for small, intermediate, and large values of k is presented.

#### I. INTRODUCTION

It has proved possible to relate many of the important properties of metals to a model in which the ions are replaced by a uniform distribution of positive charge and the conduction electrons are treated as a Fermi gas (which for metals under normal conditions is highly degenerate). Much has been learned by ignoring the Coulomb interactions between the electrons, but in recent years efforts have been made to include these interactions in the theory. Many such efforts have been focused on calculating the frequency- and wave-vector-dependent dielectric response (or screening) function  $\epsilon(\mathbf{k}, \omega)$ , because this function is the key to understanding many of the properties of metals – including those related to transport phenomena.

It is well known that the expression for  $\epsilon(\vec{k}, \omega)$ first given by Lindhard, <sup>1</sup> which can be obtained by making the random-phase approximation<sup>2,3</sup> (RPA), leads to some unphysical features of the pair distribution function in the range of metallic densities  $(2 \le r_s \le 5)$ . In a classic paper<sup>4</sup> Hubbard proposed to replace the Lindhard expression

$$1 - 1/\epsilon(\vec{k}, \omega) = Q_0(\vec{k}, \omega) / [1 + Q_0(\vec{k}, \omega)] \qquad (1.1)$$

by the more general (and hopefully more accurate) expression

$$1 - \frac{1}{\epsilon(\vec{k},\omega)} = \frac{Q_0(\vec{k},\omega)}{1 + [1 - G(\vec{k})]Q_0(\vec{k},\omega)} , \qquad (1.2)$$

where

$$Q_0(\vec{\mathbf{k}},\,\omega) = 4\lambda^2 F_0(\vec{\mathbf{k}},\,\omega)/k^2 , \qquad (1.3)$$

with

$$\lambda^{2} = (\pi a_{0}k_{f})^{-1} = \alpha r_{s}/\pi ;$$
  
$$\alpha = (4/9\pi)^{1/3}, \qquad F_{0}(\vec{k}, \omega)$$

is the polarizability of the free-electron gas. The function  $G(\vec{k})$  appearing in (1.2) takes into account exchange and correlation effects; Hubbard proposed for it the form

$$G(\vec{\mathbf{k}}) = \frac{1}{2} \left[ \frac{k^2}{(k^2 + k_f^2)} \right], \qquad (1.4)$$

with  $k_j$  the Fermi momentum. Many other forms of  $G(\vec{k})$  have since been proposed (for a review see Geldart and Vosko<sup>5</sup> and Shaw<sup>6</sup>), but we shall refer particularly to one suggested by Singwi, Tosi, Land, and Sjölander<sup>7-9</sup> (STLS). STLS arrived at an expression formally equivalent to (1. 2) by an equation-of-motion method which relates  $G(\vec{k})$ ,  $S(\vec{k})$  (the static form factor), and  $\epsilon(\vec{k}, \omega)$  self-consistently.

In a recent paper  $Shaw^{6}$  has emphasized that calculations of metallic properties depend strongly on the form of  $G(\vec{k})$ ; in addition, using the STLS results he has derived two important relations directly connecting  $G(\vec{k})$  with  $g(\vec{r})$ , the pair-distribution function. One key result of his paper is the relation<sup>10</sup>  $G(\infty) = 1 - g(0)$  which necessarily implies for the asymptotic value  $G(\infty)$  of G(k):

$$\frac{1}{2} \le G(\infty) \le 1. \tag{1.5}$$

The  $G(\vec{k})$  determined by the self-consistent procedures of STLS depends on  $r_s$ . As calculated in Ref. 7 (STLS I), it satisfies the condition (1.5) for  $r_s \leq 5$ ; as calculated in Ref. 9 (STLS III) – where the procedure of STLS I is modified and the resulting G(k) is in better accord with the compressibility sum rule – it satisfies the condition (1.5) for a smaller range of values.

In the present paper, starting from "first principles", we derive a general expression for  $\epsilon(\vec{k}, \omega)$ which turns out to be closely related to but more general than (1.2). In the static limit  $\omega = 0$ , our expression is also a functional of  $G(\vec{k})$ , and we obtain for  $G(\vec{k})$  an expression containing no adjustable parameters which in addition to having an asymptotic limit satisfying the condition (1.5) also satisfies the compressibility sum rule.<sup>11</sup> As will be seen our calculation is based on a straightforward method for decoupling and solving the equations of motion for the time-transformed Green's functions suggested by recent work of Tahir-Kehli and Jarret.<sup>12</sup> This method possesses the special virtue that it conserves the frequency moments of all the spectral functions involved.

# II. GENERAL THEORY

It is well known<sup>13</sup> that the theory of linear dissipative processes yields for the dielectric response function

$$1 - 1/\epsilon(\vec{k}, \omega) = v_{\vec{k}} \langle \langle \rho_{\vec{k}}(t); \rho_{\vec{k}}^{\dagger}(0) \rangle \rangle_{E=\omega}^{\text{ret}} = v_{\vec{k}} \mathcal{G}(\vec{k}, \omega), \quad (2.1)$$

where, as in Ref. 13, the symbol  $\langle\langle \mathbf{G}(t); \mathbf{G}(t') \rangle\rangle_{E=\omega}^{set}$  stands for the Fourier transform with respect to time of the double-time-retarded Green's function,

$$G_{r} = i\theta(t - t')\langle [\alpha(t), \mathfrak{B}(t')] \rangle ,$$
  

$$\rho_{\vec{k}}(t) = \sum_{\vec{q},\sigma} a_{\vec{q},\sigma}^{\dagger}(t) a_{\vec{k}+\vec{q},\sigma}(t) ,$$
(2.2)

with  $a^{\dagger}$  and *a* Fermi creation and annihilation operators in the Heisenberg representation and  $v_{\vec{k}} = 4\pi e^2/k^2$ . We may write Eq. (2.1) as

$$1 - \frac{1}{\epsilon(\vec{k},\omega)} = v_{\vec{k}} \sum_{\vec{q}_1\sigma_1,\vec{q}_2\sigma_2} \langle \langle a_{\vec{q}_1,\sigma_1}^{\dagger}(t)a_{\vec{k}+\vec{q}_1,\sigma_1}(t); a_{\vec{k}+\vec{q}_2,\sigma_2}^{\dagger}(0)a_{\vec{q}_2,\vec{\sigma}_2}(0) \rangle_{E=\omega}^{\text{ret}} = v_{\vec{k}} \sum_{\vec{q}_1\sigma_1,\vec{q}_2\sigma_2} F_{\vec{q}_1\sigma_1,\vec{q}_2\sigma_2}(\vec{k},\omega) , \qquad (2.3)$$

with  $F_{\vec{q}_1\sigma_1;\vec{q}_2\sigma_2}(\vec{k},\omega)$  the Fourier transform with respect to time of

$$F_{\vec{\mathfrak{q}}_{1}\sigma_{1};\vec{\mathfrak{q}}_{2}\sigma_{2}}(\vec{k},t) = \langle \langle a^{\dagger}_{\vec{\mathfrak{q}}_{1}\sigma_{1}}(t)a_{\vec{k}+\vec{\mathfrak{q}}_{1},\sigma_{1}}(t); a^{\dagger}_{\vec{k}+\vec{\mathfrak{q}}_{2},\sigma_{2}}(0)a_{\vec{\mathfrak{q}}_{2},\sigma_{2}}(0) \rangle \rangle^{\operatorname{ret}}$$

$$(2,4)$$

By differentiating Eq. (2.4) with respect to time we obtain

$$\begin{split} i\frac{d}{dt} F_{\vec{\mathfrak{q}}_{1}\sigma_{1},\vec{\mathfrak{q}}_{2}\sigma_{2}}(\vec{k},t) \\ &= -\delta(t) \langle [a_{\vec{\mathfrak{q}}_{1},\sigma_{1}}^{\dagger}(t)a_{\vec{k}+\vec{\mathfrak{q}}_{1},\sigma_{1}}(t), a_{\vec{k}+\vec{\mathfrak{q}}_{2},\sigma_{2}}^{\dagger}(0)a_{\vec{\mathfrak{q}}_{2}\sigma_{2}}(0)] \rangle \end{split}$$

$$-\langle \langle [H, a^{\dagger}_{\tilde{\mathfrak{a}}_{1},\sigma_{1}}(t)a_{\tilde{\mathfrak{k}}+\tilde{\mathfrak{a}}_{1},\sigma_{1}}(t)]; a^{\dagger}_{\tilde{\mathfrak{k}}+\tilde{\mathfrak{a}}_{2},\sigma_{2}}(0)a_{\tilde{\mathfrak{a}}_{2},\sigma_{2}}(0)\rangle \rangle ,$$
(2.5)

where H is the usual Hamiltonian

$$\begin{split} H &= \sum_{\vec{\mathfrak{p}},\sigma} \frac{\hbar^2 p^2}{2m} a_{\vec{\mathfrak{p}},\sigma}^{\dagger} a_{\vec{\mathfrak{p}},\sigma}^{\dagger} \\ &+ \sum_{\vec{k}'\neq 0; \ \vec{s}, \vec{t},\sigma,\sigma'} \frac{1}{2} v_{\vec{k}'} a_{\vec{k}',\sigma\sigma}^{\dagger} a_{\vec{t}-\vec{k}'\sigma'}^{\dagger} a_{\vec{t},\sigma'}^{\dagger} a_{\vec{s},\sigma}^{\dagger} = H_0 + H_1 \ . \end{split}$$

$$(2.6)$$

For a completely degenerate gas it is easily shown that

$$i \frac{d}{dt} F_{\vec{\mathfrak{q}}_{1}\sigma_{1},\vec{\mathfrak{q}}_{2}\sigma_{2}}(t) = \delta(t)(n_{\vec{k}+\vec{\mathfrak{q}}_{1},\sigma_{1}} - n_{\vec{\mathfrak{q}}_{1},\sigma_{1}})\delta_{\sigma_{1},\sigma_{2}}\delta_{\vec{\mathfrak{q}}_{1}\vec{\mathfrak{q}}_{2}} + \omega(\vec{\mathfrak{q}}_{1},\vec{k}) F_{\vec{\mathfrak{q}}_{1}\sigma_{1},\vec{\mathfrak{q}}_{2}\sigma_{2}}(t) + \sum_{\vec{s},\vec{k}'\sigma_{1}\sigma_{2}} v_{\vec{k}'} \langle \langle (a_{\vec{\mathfrak{q}}_{1},\sigma_{1}}^{\dagger}(t)a_{\vec{k}'+\vec{s},\sigma_{1}}^{\dagger}(t)a_{\vec{\mathfrak{q}}_{1}+\vec{k},\vec{s}',\sigma_{1}}(t)a_{\vec{\mathfrak{q}}_{1}+\vec{k},\vec{s}',\sigma_{1}}(t) - a_{\vec{\mathfrak{q}}_{1}+\vec{k},\vec{s}',\sigma_{1}}(t)a_{\vec{\mathfrak{q}}_{1}+\vec{k},\vec{s}',\sigma_{1}}(t)a_{\vec{\mathfrak{q}}_{1}+\vec{k},\sigma_{1}}(t)); a_{\vec{k}+\vec{\mathfrak{q}}_{2},\sigma_{2}}^{\dagger}(0)a_{\vec{\mathfrak{q}}_{2},\sigma_{2}}(0) \rangle \rangle^{\text{ret}}, \qquad (2.7)$$

$$\omega(\mathbf{\bar{q}},\mathbf{k}) = (\hbar^2/2m)[(\mathbf{\bar{q}}+\mathbf{k})^2 - \mathbf{\bar{q}}^2]$$

and  $n_{\bar{d}}$  is the Fermi distribution function, which for a degenerate gas is a step function. Taking the Fourier transform of both sides of Eq. (2, 7)and assuming that the interaction is switched on slowly (adiabatic assumption) leads to

$$[\omega - \omega(\vec{q}_{1}, \mathbf{k}) + i\delta] F_{\vec{q}_{1}\sigma_{1};\vec{q}_{2}\sigma_{2}}$$
  
=  $(n_{\vec{k}+\vec{q}_{1},\sigma_{1}} - n_{\vec{q}_{1},\sigma_{1}})\delta_{\sigma_{1},\sigma_{2}}\delta_{\vec{q}_{1},\vec{q}_{2}} + \sum_{\vec{s}_{1}\vec{k}'} F_{\vec{s},\vec{k}',\vec{q}_{1},\vec{q}_{2},\sigma_{1},\sigma_{2}}^{(1)},$   
(2.8)

with  $F^{(1)}$  given by the Fourier transform of the second term in the right-hand side of Eq. (2.7). It is to be noted that if we decouple Eq. (2.8) by putting k = -k' and then pairing off the equal momentum operators by setting  $\langle a_{\bar{\mathfrak{q}},\sigma}^{\dagger}a_{\bar{\mathfrak{q}},\sigma}\rangle = n_{\bar{\mathfrak{q}},\sigma}$ , we obtain

$$\begin{split} [\omega - \omega(\vec{q}_{1}, \vec{k}) + i\delta] F_{\vec{q}_{1}, \sigma_{1};\vec{q}_{2}\sigma_{2}} &- v_{\vec{k}}(n_{\vec{k}+\vec{q}_{1},\sigma_{1}} - n_{\vec{q}_{1},\sigma_{1}}) \\ &= (n_{\vec{k}+\vec{q}_{1},\sigma_{1}} - n_{\vec{q}_{1},\sigma_{1}})\delta_{\sigma_{1},\sigma_{2}}\delta_{\vec{q}_{1},\vec{q}_{2}} \\ &\times \sum_{\vec{s},\sigma_{1}} F_{\vec{s},\sigma_{1},\vec{q}_{2}\sigma_{2}}, \end{split}$$
(2.9)

which leads directly to the RPA result. Thus, it is reasonable to expect that use of a less crude method for decoupling will yield better results than can be obtained with RPA.

Tahir-Kehli and Jarrett<sup>12</sup> proposed that one decouple by expressing  $g^{(n)}(E)$ , the Fourier time transform of a higher-order Green's function as a sum of the lower-order ones with appropriately chosen coefficients.

O(n-1)

$$S^{(n)}(E) = A_{n-1}S^{(n-1)}(E)$$
  
+ $A_{n-2}S^{(n-2)}(E) + \cdots + A_0S^{(0)}(E).$  (2.10)

We determine the A coefficients by requiring conservation of the first *n*-frequency moments  $\overline{\omega}^{(n)}$  of the spectral function associated with  $G^{(n)}$ . [As applied in the present context, this procedure differs significantly from any considered in Ref. 12; comments as to its motivation and justification will be found after Eqs. (2.12) and (2.14).] That is, if we restrict ourselves to calculating  $g^{(1)}$ , we will have

$$g^{(1)} = A_0 g^{(0)}$$

where

$$A_0 = \int_{-\infty}^{+\infty} J^{(1)}(\omega) \omega d\omega / \int_{-\infty}^{+\infty} J^{(0)}(\omega) \omega d\omega$$

$$=\overline{\omega}^{(1)}\{g^{(1)}\}/\overline{\omega}^{(1)}\{g^{(0)}\},\qquad(2.11)$$

with  $J^{(0)}(\omega)$  and  $J^{(1)}(\omega)$  spectral functions corresponding, respectively, to  $g^{(0)}$  and  $g^{(1)}$ , and  $\overline{\omega}^{(1)}$  $\{\mathbf{g}^{(1)}\}\$  and  $\overline{\omega}^{(1)}\{\mathbf{g}^{(0)}\}\$  first-frequency moments of  $J^{(1)}(\omega)$  and  $J^{(0)}(\omega)$ . It should be noted that in order to calculate  $\overline{\omega}^{(1)}\{g^{(1)}\}$  and  $\overline{\omega}^{(1)}\{g^{(0)}\}$  it is not necessary to know explicitly  $J^{(1)}(\omega)$  and  $J^{(0)}(\omega)$ , as, if we have the Green's function

$$g = \langle \langle \alpha(t); \alpha(t') \rangle \rangle$$

with spectral function  $J(\omega)$ , then

$$\overline{\omega}^{(n)}[\underline{G}] = \int_{-\infty}^{+\infty} J(\omega)\omega^n d\omega$$
$$= \lim_{t \to t'} \left\langle \left[ \left( i \frac{d}{dt} \right)^{n-p} \mathbf{a}(t), \left( -i \frac{d}{dt} \right)^p \mathbf{B}(t') \right] \right\rangle. \quad (2.12)$$

We note that this method will be very good for large  $\omega$ , and not worse than other decoupling methods for small  $\omega$ .<sup>14</sup> Before applying this method to our problem, we modify slightly Eq. (2.8). As we are primarily interested in

$$\mathcal{G}(\vec{\mathbf{k}},\,\omega) = \sum_{\vec{\mathfrak{q}}_1,\,\sigma_1,\,\vec{\mathfrak{q}}_2,\,\sigma_2} F_{\vec{\mathfrak{q}}_1,\,\sigma_1;\,\vec{\mathfrak{q}}_2,\,\sigma_2}(\vec{\mathbf{k}},\,\omega) \ ,$$

we sum both sides of Eq. (2.8) over  $\overline{q}_2$  and  $\sigma_2$ to obtain

$$\begin{split} [\omega - \omega(\vec{\mathbf{q}}_1, \vec{\mathbf{k}}) + i\delta] \mathcal{F}_{\vec{\mathbf{q}}_1, \sigma_1}(\vec{\mathbf{k}}, \omega) \\ &= (n_{\vec{\mathbf{k}} + \vec{\mathbf{q}}_1, \sigma_1} - n_{\vec{\mathbf{q}}_1, \sigma_1}) + \mathcal{F}_{\vec{\mathbf{q}}_1, \sigma_1}^{(1)}(\vec{\mathbf{k}}, \omega), \end{split}$$
(2.13)

where

$$\mathfrak{F}_{\mathfrak{\tilde{d}}_{1},\mathfrak{\sigma}_{1}}(\mathbf{\bar{k}},\,\omega) = \sum_{\mathfrak{\tilde{d}}_{2},\mathfrak{\sigma}_{2}} F_{\mathfrak{\tilde{d}}_{1},\mathfrak{\sigma}_{1}};\mathfrak{\tilde{d}}_{2},\mathfrak{\sigma}_{2}}$$

and

$$\mathcal{F}^{(1)}_{\vec{\mathfrak{q}}_{1},\sigma_{1}} = \sum_{\vec{\mathfrak{q}}_{2},\vec{\mathfrak{s}},\vec{\mathfrak{k}}';\sigma_{2}} F^{(1)}_{\vec{\mathfrak{s}},\vec{\mathfrak{k}}',\vec{\mathfrak{q}}_{1}\sigma_{1};\vec{\mathfrak{q}}_{2}\sigma_{2}} \ .$$

Now, observing that the RPA decoupling expresses  $\mathfrak{F}_{\mathfrak{q}_1,\sigma_1}^{(1)}$  as a linear combination of all the F's, i.e.,

$$\mathfrak{F}_{\mathfrak{q}_{1},\mathfrak{o}_{1}}^{(1)}(\vec{\mathbf{k}},\,\omega) = A_{\mathfrak{q}_{1},\mathfrak{o}_{1}} \sum_{\vec{m},\sigma} \mathfrak{F}_{\vec{m},\sigma}(\vec{\mathbf{k}},\,\omega), \qquad (2.14)$$

we try to express our  $\mathfrak{F}^{(1)}$  in the same way (2.14) with  $A_{\mathfrak{q}_1,\mathfrak{o}_1}$  to be determined by Eq. (2.11) via Eq. (2.12). Determining the set of  $A_{\mathfrak{q}_1\mathfrak{o}}$  in this way is equivalent to requiring conservation of the integral over all frequencies of the spectral density associated with  $\mathfrak{F}^{(1)}$ . As is shown below, this procedure results in a  $G(\vec{k})$  with many features which correspond to the requirements of physics. However, at present it is difficult to provide an *a priori* justification for the conservation requirement based on anything other than its heuristic value. It should be noted that, as is clear from Eq. (2.14), our

decoupling procedure differs from those discussed in Ref. 12 in that we relate one  $\bar{q}$ ,  $\sigma$  component of  $\mathfrak{F}^{(1)}$  to the *sum* of all the components of  $\mathfrak{F}$  rather than to one only.

Noting that

$$\sum_{\vec{m},\sigma} \mathfrak{F}_{\vec{m},\sigma} = \mathfrak{g}(\vec{k},\omega) ,$$

we substitute Eq. (2.14) into Eq. (2.13) to obtain

$$\mathfrak{F}_{\mathfrak{q}_{1},\mathfrak{\sigma}_{1}} = \frac{(n_{\tilde{k}+\tilde{\mathfrak{q}}_{1},\mathfrak{\sigma}_{1}}-n_{\tilde{\mathfrak{q}}_{1},\mathfrak{q}_{1}})+A_{\tilde{\mathfrak{q}}_{1},\mathfrak{\sigma}}G(\tilde{k},\omega)}{\omega-\omega(\tilde{\mathfrak{q}}_{1},\tilde{k})+i\delta} ; \qquad (2.15)$$

then summing both sides over  $\dot{q}_1, \sigma_1$  leads to

$$S(\vec{k}, \omega) = \sum_{\vec{q}_1, \sigma_1} \frac{n_{\vec{k}+\vec{q}_1, \sigma_1} - n_{\vec{q}_1\sigma_1}}{\omega - \omega(\vec{q}_1, \vec{k}) + i\delta} + S(\vec{k}, \omega) \sum_{\vec{q}_1\sigma_1} \frac{A_{\vec{q}_1, \sigma_1}}{\omega - \omega(\vec{q}_1, \vec{k}) + i\delta}$$
(2.16)

Solving for  $\mathfrak{S}(\mathbf{k}, \omega)$  and substituting the expression

thus obtained back into (2.1) we arrive at the final result

$$1 - \frac{1}{\epsilon(\vec{k}, \omega)} = v_{\vec{k}} \sum_{\vec{\mathfrak{q}}, \sigma} \frac{n_{\vec{k}+\vec{\mathfrak{q}}, \sigma}^{\ast} - n_{\vec{\mathfrak{q}}, \sigma}^{\ast}}{\omega - \omega(\vec{\mathfrak{q}}, \vec{k}) + i\delta} / \left(1 - \sum_{\vec{\mathfrak{q}}, \sigma} \frac{A_{\vec{\mathfrak{q}}, \sigma}}{\omega - \omega(\vec{\mathfrak{q}}, \vec{k}) + i\delta}\right),$$
(2.17)

which is formally equivalent to Eq. (2.1), as will be shown more explicitly in Sec. III.

III. DERIVATION OF  $A_{\mathbf{\tilde{q}}_1,\sigma_1}$ 

According to our definition of  $A_{\overline{\mathfrak{q}}_1,\sigma_1}$  and to the previously established notations, it follows that

$$A_{\mathbf{\tilde{q}}_{1},\sigma_{1}} = \overline{\omega}^{(1)} \{ \mathfrak{F}_{\mathbf{\tilde{q}}_{1},\sigma_{1}}^{(1)} \} / \overline{\omega}^{(1)} \{ \sum_{\mathbf{\tilde{q}}_{1},\sigma_{1}} \mathfrak{F}_{\mathbf{\tilde{q}}_{1},\sigma_{1}} \} , \qquad (3.1)$$

where, from Eq. (2.12),

$$\overline{\omega}^{(1)}\{\mathfrak{F}^{(1)}_{\mathfrak{q}_{1},\mathfrak{a}_{1}}\} = -\lim_{t \to 0} \sum_{\mathfrak{q}_{2}\sigma_{2},\mathfrak{s},\mathfrak{k}'} v_{\mathfrak{k}'} \langle [[H, (a_{\mathfrak{q}_{2},\sigma_{1}}^{\dagger}(t)a_{\mathfrak{k}',\mathfrak{s},\sigma_{1}}^{\dagger}(t)a_{\mathfrak{s},\sigma_{1}}^{\dagger}(t)a_{\mathfrak{q}_{1},\mathfrak{k},\mathfrak{k}',\sigma_{1}}^{\dagger}(t)a_{\mathfrak{q}_{1},\mathfrak{k}',\mathfrak{s},\sigma_{1}}^{\dagger}(t)a_{\mathfrak{q}_{1},\mathfrak{k}',\mathfrak{s},\sigma_{1}}^{\dagger}(t)a_{\mathfrak{q}_{1},\mathfrak{k}',\mathfrak{s},\sigma_{1}}^{\dagger}(t)a_{\mathfrak{q}_{1},\mathfrak{k}',\mathfrak{s},\sigma_{1}}^{\dagger}(t)a_{\mathfrak{q}_{1},\mathfrak{k}',\mathfrak{s},\sigma_{1}}^{\dagger}(t)a_{\mathfrak{q}_{1},\mathfrak{k}',\mathfrak{s},\sigma_{1}}^{\dagger}(t)a_{\mathfrak{q}_{2},\mathfrak{s},\sigma_{2}}^{\dagger}(0)a_{\mathfrak{q}_{2},\mathfrak{s},\sigma_{2}}^{\dagger}(0)]\rangle,$$

$$(3.2)$$

$$\overline{\omega}^{(1)}\left\{\sum_{\mathfrak{q}_{1}\sigma_{1}}\mathfrak{F}_{\mathfrak{q}_{1}\sigma_{1}}\right\} = -\lim_{t\to 0}\sum_{\mathfrak{q}_{1}\sigma_{1};\mathfrak{q}_{2}\sigma_{2}}\left\langle\left\{\left[H,a_{\mathfrak{q}_{1},\sigma_{1}}^{\dagger}(t)a_{k},\mathfrak{q}_{1},\sigma_{1}(t)\right], a_{k}^{\dagger},\mathfrak{q}_{2}\sigma_{2}(0)a_{\mathfrak{q}_{2}\sigma_{2}}(0)\right\}\right\rangle.$$

$$(3.3)$$

One finds after a lengthy calculation and after having discarded the terms in (3.2) coming from  $H_1$  (see Appendix A),

$$A_{\vec{\mathfrak{q}}_{1},\sigma_{1}} = -v_{\vec{\mathfrak{k}}}(n_{\vec{\mathfrak{k}}+\vec{\mathfrak{q}}_{1},\sigma_{1}} - n_{\vec{\mathfrak{q}}_{1},\sigma_{1}}) + \sum_{\vec{\mathfrak{k}}'} v_{\vec{\mathfrak{k}}'} \omega(\vec{\mathfrak{q}}_{1},\vec{\mathfrak{k}})(n_{\vec{\mathfrak{q}}_{1}+\vec{\mathfrak{k}},\sigma_{1}} - n_{\vec{\mathfrak{q}}_{1},\sigma_{1}})(n_{\vec{\mathfrak{q}}_{1}+\vec{\mathfrak{k}},\sigma_{1}} - n_{\vec{\mathfrak{q}}_{1},\sigma_{1}})/\sum_{\vec{\mathfrak{q}}_{2},\sigma_{2}} \omega(\vec{\mathfrak{q}}_{2},\vec{\mathfrak{k}})(n_{\vec{\mathfrak{k}}+\vec{\mathfrak{q}}_{2},\sigma_{2}} - n_{\vec{\mathfrak{q}}_{2},\sigma_{2}})$$
$$+ \sum_{\vec{\mathfrak{q}}_{2}} v_{\vec{\mathfrak{q}}_{1}-\vec{\mathfrak{q}}_{2}} \omega(\vec{\mathfrak{q}}_{2},\vec{\mathfrak{k}})(n_{\vec{\mathfrak{k}}+\vec{\mathfrak{q}}_{2},\sigma_{1}} - n_{\vec{\mathfrak{q}}_{2},\sigma_{2}})(n_{\vec{\mathfrak{q}}_{1}+\vec{\mathfrak{k}},\sigma_{1}} - n_{\vec{\mathfrak{q}}_{1},\sigma_{1}})/\sum_{\vec{\mathfrak{q}}_{2},\sigma_{2}} \omega(\vec{\mathfrak{q}}_{2},\vec{\mathfrak{k}})(n_{\vec{\mathfrak{k}}+\vec{\mathfrak{q}}_{2},\sigma_{2}} - n_{\vec{\mathfrak{q}}_{2},\sigma_{2}}) \quad . \tag{3.4}$$

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It should be noted at this point that the first term on the right-hand side of Eq. (3.4) is the only one retained in the RPA. It is easy to see that the remaining two terms take account of processes involving exchange: This is clear from the appearance of  $v_{\vec{a}_1-\vec{a}_2}$  in the third term, and also in the second term if it is first transformed by a change of the summation index  $\vec{k}'$  to  $\vec{q}_1 - \vec{q}_2$ . Now in order to exhibit the formal equivalence between Eqs. (2.17) and (1.2) we write the term

$$-\sum_{\vec{\mathfrak{q}}_1,\mathfrak{s}_1}\frac{A_{\vec{\mathfrak{q}}_1\mathfrak{s}_1}}{\omega-\omega(\vec{\mathfrak{q}}_1,\vec{k})+i\delta}$$

in the denominator of Eq. (2.17) as

$$\left( \sum_{\mathfrak{q}_{1}\sigma} \frac{v_{\mathfrak{k}}(n_{\mathfrak{k}+\mathfrak{q},\sigma}-n_{\mathfrak{q},\sigma})}{\omega-\omega(\tilde{\mathfrak{q}},\tilde{\mathfrak{k}})+i\delta} \right) \left[ 1 - \sum_{\mathfrak{q}_{1},\sigma_{1}} \left( \sum_{\mathfrak{q}_{2}} v_{\mathfrak{q}_{1}-\mathfrak{q}_{2}} \left[ \omega(\tilde{\mathfrak{q}}_{1}\tilde{\mathfrak{k}}) - \omega(\tilde{\mathfrak{q}}_{2},\tilde{\mathfrak{k}}) \right] (n_{\mathfrak{q}_{1}+\mathfrak{k}_{1}\sigma_{1}} - n_{\mathfrak{q}_{1},\sigma_{1}}) (n_{\mathfrak{q}_{2},\sigma_{1}} - n_{\mathfrak{q}+\mathfrak{k},\sigma}) \right] \\ \times \left\{ \sum_{\mathfrak{q}_{2}\sigma_{2}} \omega(\tilde{\mathfrak{q}}_{2},\tilde{\mathfrak{k}}) (n_{\mathfrak{k}+\mathfrak{q}_{2},\sigma_{2}} - n_{\mathfrak{q}_{2}\sigma_{2}}) [\omega - \omega(\tilde{\mathfrak{q}}_{1},\tilde{\mathfrak{k}}) + i\delta] \right\}^{-1} \right) / \sum_{\mathfrak{q},\sigma} \frac{v_{\mathfrak{k}}(n_{\mathfrak{k}+\mathfrak{q},\sigma}+n_{\mathfrak{q},\sigma})}{[\omega - \omega(\tilde{\mathfrak{q}},\tilde{\mathfrak{k}}) + i\delta]} = Q_{0}(\tilde{\mathfrak{k}},\omega) \left( 1 - \frac{P_{0}(\tilde{\mathfrak{k}},\omega)}{Q_{0}(\tilde{\mathfrak{k}},\omega)} \right) \quad , (3.5)$$

where we have used the change  $\mathbf{\vec{k}'} - \mathbf{\vec{q}_1} - \mathbf{\vec{q}_2}$  in (3. 4), and  $Q_0(\mathbf{\vec{k}}, \omega)$  is the Lindhard polarization function, while  $P_0(\mathbf{\vec{k}}, \omega)$  includes exchange and correlation effects omitted in  $Q_0(\mathbf{\vec{k}}, \omega)$ . It is now easy to recognize that, with

$$G(\vec{\mathbf{k}},\,\omega) = P_0(\vec{\mathbf{k}},\,\omega)/Q_0(\vec{\mathbf{k}},\,\omega) , \qquad (3.6)$$

Eq. (2.17) becomes

$$1 - \frac{1}{\epsilon(\vec{k}, \omega)} = \frac{Q_0(k, \omega)}{1 + Q_0(\vec{k}, \omega)[1 - G(\vec{k}, \omega)]} , \qquad (3.7)$$

which shows that in our case G depends explicitly also on  $\omega$ , and hence is a generalization of the corresponding function appearing in Eq. (1.2).

#### IV. STATIC CASE

In this paper we carry out explicit calculations for the static case, that is we specialize the general Eq. (3.7) to

$$1 - \frac{1}{\epsilon(\vec{k}, 0)} = \frac{Q_0(\vec{k}, 0)}{1 + [1 - G(\vec{k}, 0)]Q_0(\vec{k}, 0)} .$$
(4.1)

Noting that for a completely degenerate gas one obtains

$$\sum_{q_2,\sigma_2} \omega(q_2,k)(n_{k+q_2,\sigma_2} - n_{q_2,\sigma_2}) = -\frac{\hbar^2 k^2}{m} \frac{k_f^3}{3\pi^2} \quad , \quad (4.2)$$

and setting  $\omega = 0$ , we may write

$$P_{0}(k, 0) = -\frac{2m(3\pi^{2})}{\hbar^{2}k^{2}k_{F}^{3}} \sum_{\mathfrak{d}_{1},\mathfrak{d}_{2}} v_{\mathfrak{d}_{1}-\mathfrak{d}_{2}} \left(1 - \frac{\omega(\mathfrak{d}_{2}, \tilde{k})}{\omega(\mathfrak{d}_{1}, \tilde{k})}\right) \times (n_{\mathfrak{d}_{1}+\mathfrak{k}} - n_{\mathfrak{d}_{1}})(n_{\mathfrak{k}+\mathfrak{d}_{2}} - n_{\mathfrak{d}_{2}}) \quad .$$
(4.3)

And writing

$$(n_{\overline{\mathfrak{q}}_{1}+\overline{\mathfrak{k}}} - n_{\overline{\mathfrak{q}}_{1}})(n_{\overline{\mathfrak{k}}+\overline{\mathfrak{q}}_{2}} - n_{\overline{\mathfrak{q}}_{2}})$$

$$= \theta_{\langle}(\overline{\mathfrak{q}}_{1} + \overline{\mathfrak{k}})\theta_{\rangle}(\overline{\mathfrak{q}}_{1})\theta_{\langle}(\overline{\mathfrak{k}} + \overline{\mathfrak{q}}_{2})\theta_{\rangle}(\overline{\mathfrak{q}}_{2})$$

$$- \theta_{\rangle}(\overline{\mathfrak{q}}_{1} + \overline{\mathfrak{k}})\theta_{\langle}(\overline{\mathfrak{q}}_{1})\theta_{\langle}(\overline{\mathfrak{q}}_{2} + \overline{\mathfrak{k}})\theta_{\rangle}(\overline{\mathfrak{q}}_{2})$$

$$-\theta_{\zeta}(\vec{q}_{1}+\vec{k})\theta_{\zeta}(\vec{q}_{1})\theta_{\zeta}(\vec{q}_{2}+\vec{k})\theta_{\zeta}(\vec{q}_{2})$$
  
+ $\theta_{\zeta}(\vec{q}_{1}+\vec{k})\theta_{\zeta}(\vec{q}_{1})\theta_{\zeta}(\vec{q}_{2}+\vec{k})\theta_{\zeta}(\vec{q}_{2}), \quad (4.4)$ 

$$\theta_{>}(P) = \begin{cases} 1, & P > k_f \\ 0, & P < k_f \end{cases}$$
$$\theta_{<}(P) = 1 - \theta_{>}(P) ,$$

we see that for carrying out the summation a technique similar to that used by Geldart and Taylor<sup>15</sup> is useful: That is, first of all we change  $\tilde{q}$  into  $-\tilde{q} - \tilde{k}$  whenever we have  $\theta_{\langle}(\tilde{q} + \tilde{k})$ ; so doing one obtains

$$P_{0}(\vec{\mathbf{k}}, 0) = -\frac{4 \cdot 4\pi e^{2} 3\pi^{2} m}{\hbar^{2} k^{2} k_{f}^{3}} \sum_{\vec{\mathbf{q}}_{1}, \vec{\mathbf{q}}_{2}} \left[ \left( 1 - \frac{2\vec{\mathbf{q}}_{2} \cdot \vec{\mathbf{k}} + k^{2}}{2\vec{\mathbf{q}}_{1} \cdot \vec{\mathbf{k}} + k^{2}} \right) \right]$$

$$\times \frac{1}{|\vec{\mathbf{q}}_{1} - \vec{\mathbf{q}}_{2}|^{2}} - \left( 1 + \frac{2\vec{\mathbf{q}}_{2} \cdot \vec{\mathbf{k}} + k^{2}}{2\vec{\mathbf{q}}_{1} \cdot \vec{\mathbf{k}} + k^{2}} \right) \frac{1}{|\vec{\mathbf{q}}_{1} + \vec{\mathbf{q}}_{2} + \vec{\mathbf{k}}|^{2}}$$

$$\times \theta_{\zeta}(\vec{\mathbf{q}}_{1}) \theta_{\zeta}(\vec{\mathbf{q}}_{2}) \theta_{\zeta}(\vec{\mathbf{q}}_{1} + \vec{\mathbf{k}}) \theta_{\zeta}(\vec{\mathbf{q}}_{2} + \vec{\mathbf{k}}) . \quad (4.5)$$

We perform now the transformation

$$\vec{q}_1 = \vec{q}_1 - \frac{1}{2}\vec{k}$$
,  $\vec{q}_2 = \vec{q}_2 - \frac{1}{2}\vec{k}$ ,

obtaining

$$P_{0}(\mathbf{k}, 0) = -\frac{48\pi^{3}me^{2}}{\hbar^{2}k^{2}k_{f}^{3}} \sum_{\vec{q}_{1}\vec{q}_{2}} \left[ \left( 1 - \frac{\vec{q}_{2} \cdot \vec{k}}{\vec{q}_{1} \cdot \vec{k}} \right) \frac{1}{|\vec{q}_{1} - \vec{q}_{2}|^{2}} - \left( 1 + \frac{\vec{q}_{2} \cdot \vec{k}}{\vec{q}_{1} \cdot \vec{k}} \right) \frac{1}{|\vec{q}_{1} + \vec{q}_{2}|^{2}} \right] \theta_{\zeta}(\vec{q}_{1} - \frac{1}{2}\vec{k}) \\ \times \theta_{\zeta}(\vec{q}_{2} - \frac{1}{2}\vec{k})\theta_{\zeta}(\vec{q}_{1} + \frac{1}{2}\vec{k})\theta_{\zeta}(\vec{q}_{2} + \frac{1}{2}\vec{k}) . \quad (4.6)$$

And finally we symmetrize the sum in (4.6) with respect to  $q_1$  and  $q_2$  and divide by 2, obtaining the form

$$P_{0}(k, 0) = \frac{24\pi^{3}me^{2}}{\hbar^{2}k^{2}k_{f}^{3}} \sum_{\vec{q}_{1}\vec{q}_{2}} \left( \frac{\left[(\vec{q}_{1} - \vec{q}_{2}) \cdot \vec{k}\right]^{2}}{|\vec{q}_{1} - \vec{q}_{2}|^{2}} + \frac{\left[(\vec{q}_{1} + \vec{q}_{2}) \cdot \vec{k}\right]^{2}}{|\vec{q}_{1} + \vec{q}_{2}|^{2}} \right) \frac{\theta_{\zeta}(\vec{q}_{1} - \frac{1}{2}\vec{k})\theta_{\zeta}(\vec{q}_{2} - \frac{1}{2}\vec{k})\theta_{\zeta}(\vec{q}_{1} + \frac{1}{2}\vec{k})\theta_{\zeta}(\vec{q}_{2} + \frac{1}{2}\vec{k})$$

This expression is now conveniently written in order to change the sums into integrals; then we express the momenta in units of  $k_f$  so as to have

$$P_0(k, 0) = \frac{3}{8} (\alpha r_s / \pi^3) (F^- + F^+) , \qquad (4.8)$$

where

$$F^{\pm} = \frac{1}{k^{2}} \int d^{3}\vec{q}_{1} \int d^{3}\vec{q}_{2} \frac{\left[ (\vec{q}_{1} \pm \vec{q}_{2}) \cdot \vec{k} \right]^{2}}{|\vec{q}_{1} \pm \vec{q}_{2}|^{2}} \frac{\theta_{\langle} (\vec{q}_{1} - \frac{1}{2}\vec{k})\theta_{\langle} (\vec{q}_{2} - \frac{1}{2}\vec{k})\theta_{\rangle} (\vec{q}_{1} + \frac{1}{2}\vec{k})\theta_{\rangle} (\vec{q}_{2} + \frac{1}{2}\vec{k})}{(\vec{q}_{1} \cdot \vec{k})(\vec{q}_{2} \cdot \vec{k})}$$

$$(4.9)$$

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The Coulomb singularity in Eq. (4.9) is explicitly cancelled by the numerator, and the resulting in-

tegral is smooth. The limits of integration implied by the product of  $\theta$ 's may be included in  $x_1, x_2$ , the cosines of the angles between  $\bar{q}_1, \bar{q}_2$ , and  $\bar{k}$ , and in  $q_1, q_2$  so that the integration over  $d\varphi_1$  and  $d\varphi_2$  may be carried out analytically to give<sup>15</sup>

$$\int_{0}^{2\pi} d\varphi_{1} \int_{0}^{2\pi} d\varphi_{2} \frac{1}{|\vec{q}_{1} + \vec{q}_{2}|^{2}} = \frac{4\pi^{2}}{[R_{a_{1}a_{2}}^{*}(x_{1}x_{2})]^{1/2}},$$
(4.10)

with

$$0 \le x \le 1$$
  
- $\frac{1}{2}kx + [1 + \frac{1}{4}k^2(x^2 - 1)]^{1/2} \le q \le \frac{1}{2}kx + [1 + \frac{1}{4}k^2(x^2 - 1)]^{1/2}$   
 $\left(1 - \frac{4}{k^2}\right)^{1/2} \le x \le 1$   
 $\frac{1}{2}kx - [1 + \frac{1}{4}k^2(x^2 - 1)]^{1/2} \le q \le \frac{1}{2}kx + [1 + \frac{1}{4}k^2(x^2 - 1)]^{1/2}$ 

With rescaling of the variables as in Ref. 15 it: is easily seen that the two integrals are reduced to

$$F^{\pm} = H\pi^2 \int_0^1 dx_1 \int_0^1 dx_2 \int_0^1 ds_1 \int_0^1 ds_2 \frac{q_1 q_2 (q_1 x_1 \pm q_2 x_2)^2}{[R_{q_1 q_2}^{\pm}(x_1, x_2)]^{1/2}},$$
(4.13)

with

$$q = +kx(s - \frac{1}{2}) + \left[1 + \frac{1}{4}k^2(x^2 - 1)\right]^{1/2} \quad \text{for } k \le 2$$

and

$$F^{\pm} = \frac{4\pi^2}{k^2} \left[ 1 - \left( 1 - \frac{4}{k^2} \right)^{1/2} \right] \int_0^1 dy_1 \int_0^1 dy_2 \int_0^1 ds_1$$
$$\times \int_0^1 ds_2 \quad 4 \left[ 1 + \frac{1}{4}k^2 (x_1^2 - 1) \right]^{1/2} \left[ 1 + \frac{1}{4}k^2 (x_2^2 - 1) \right]^{1/2}$$

$$\times \frac{q_1 q_2 (q_1 x_1 \pm q_2 x_2)^2}{x_1 x_2 [R_{q_1 q_2}^{\pm}(x_1, x_2)]^{1/2}} , \qquad (4.14)$$

with

$$x = y \left(1 - \frac{4}{k^2}\right)^{1/2} + \left(1 - \frac{4}{k^2}\right)^{1/2}$$

and

$$q = \frac{1}{2}kx + (s-1)[1 + \frac{1}{4}k^2(x^2-1)]^{1/2} \quad \text{for } k \ge 2.$$

We recall that

$$G(k, 0) = \frac{3}{8} \frac{\alpha \gamma_s}{\pi^2} \frac{(F^+ + F^+)}{Q_0(k, 0)} ; \qquad (4.15)$$

the explicit form of  $Q_0(k, 0)$  is

$$Q_0(k, 0) = \frac{4\alpha r_s}{k^2 \pi} F_0(k, 0) ,$$

where

$$R_{q_1q_2}^{\pm} = (q_1^2 - q_2^2)^2 + 4q_1q_2[q_1q_2(x_1 \pm x_2)^2 \pm x_1x_2(q_1 - q_2)^2] .$$
(4.11)

The factor

$$\theta_{\mathsf{c}}(\mathbf{\bar{q}}_1 - \frac{1}{2\mathbf{\bar{k}}})\theta_{\mathsf{c}}(\mathbf{\bar{q}}_2 - \frac{1}{2\mathbf{\bar{k}}})\theta_{\mathsf{c}}(\mathbf{\bar{q}}_1 + \frac{1}{2\mathbf{\bar{k}}})\theta_{\mathsf{c}}(\mathbf{\bar{q}}_2 + \frac{1}{2\mathbf{\bar{k}}})$$

defines two different k regions for the domain of integration. Replacing  $x_1$  or  $x_2$  by x and  $q_1$  or  $q_2$  by q we have

$$\begin{cases} k \leq 2, \\ k \leq 2, \\ k \leq 2. \end{cases}$$

$$(4.12)$$

$$F_0(k, 0) = \frac{1}{2} + \frac{1}{2k} \left(1 - \frac{1}{4}k^2\right) \ln \left|\frac{k+2}{k-2}\right| ; \qquad (4.16)$$

k is in units of  $k_F$  as usual.

### V. COMPRESSIBILITY

One of the most important and distinctive results of this calculation concerns the limit of  $G(k)/k^2$  for small k. From the compressibility sum rule, <sup>16</sup>

$$\lim k^2 \epsilon(k, 0) = 4\lambda^2 (C/C_0) \text{ as } k \to 0,$$

where c and  $c_0$  are respectively the compressibility of the interacting gas and of the free-electron gas.



FIG. 1. Ratio of free electron to interacting electron compressibilities  $C_0/C$ , versus  $r_s$ . Curves 1, 2, and 3 are, respectively, the results of RPA, Hubbard (same as STLS<sup>7</sup>), and improved STLS.<sup>8,9</sup> Curve 5 shows the results of the present paper; curve 4 gives the values obtained by differentiation of the energy.

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0.76213

TABLE I. Values of G(k). G(k)G(k)k k 0.00251 0.1 2.3 0.72756 0.01001 0.724160.2 2.4 0.3 0.022572.5 0.72275 0.04021 2.6 0,72254 0.40.5 0.06296 2.7 0.72309 0.6 0.09081 2.8 0.724180.7 0.12374 2.9 0.72558 0.8 0.16171 3.0 0.72710 0.9 0.728730.204613.11.0 0.252313.2 0.73037 0.304603.3 0.73199 1.1 0.36117 1.23.4 0.73355 0.42162 3.5 0.73503 1.30.48534 0.73644 1.4 3.6 0.737761.5 0.551473.7 0,61871 0.73900 1.6 3.8 0.68493 0.74016 1.73.9 1.8 0.74631 4.00.741241.9 0.79435 5.0 0.74886 1.95 0.80667 6.0 0.753007.0 0.78999 0.755472. 2.1 0.74824 8.0 0.75705  $2 \times 10^3$ 

Equation (5.1) implies

0.73439

$$C_0/C = 1 - 4\gamma\lambda^2, \qquad (5.2)$$

where

2.2

 $\gamma = \lim [G(k)/k^2]$  as  $k \to 0$ . (5.3)

In our case, as is shown in Appendix B, we obtain

$$\gamma = \frac{1}{4} \,. \tag{5.4}$$

This value gives compressibilities in close agreement with those tabulated by Rice.<sup>17</sup> According to Hedin and Lundqvist<sup>10</sup> in fact,  $\gamma \approx \frac{1}{4}$  is obtained from an exact calculation of the compressibility. On the other hand both STLS<sup>7</sup> and Hubbard failed to obtain this result, and in order to calculate the compressibility they had to use the thermodynamic definition of  $C/C_0$ . The improved G(k) of  $STLS^{8,9}$  leads to better results as indicated in Fig. 1.

In Fig. 1 values of the compressibility obtained from various calculations of  $\epsilon(\vec{k}, 0)$  via Eq. (5.1) are compared with values obtained from the second derivative of the energy, which are usually regarded as the most reliable because of the good agreement in the results obtained by several authors using different approximations. It is clear that of the compressibilities derived using the sum rule (5.1), ours agree best with the energy-derived compressibilities. The fact that our calculation leads directly to the value  $\gamma = \frac{1}{4}$  suggests that at least for small k it takes account of exchange effects as well as do other treatments devoted explicitly to their evaluation.

#### VI. RESULTS AND REMARKS

Integrals (4.13) and (4.15) were evaluated numerically; the results obtained for

$$G(k, 0) = P_0(k, 0) / Q_0(k, 0)$$
 (6.1)

are given in Table I. This table gives for the asymptotic value of G(k, 0) about 0.762:

$$\lim G(k, 0) = 0.762$$
 as  $k \to \infty$ , (6.2)

which agrees with (1.5), confirming<sup>6</sup> that the method used here takes into account not only statisical effects, but also some of the effects of the Coulomb repulsion between the electrons.

In Fig. 2 we compare the values of the quantity  $G(k)/k^2$  obtained in this paper with the corresponding results of STLS.<sup>7</sup> This quantity plays the role of an effective electron-electron interaction; Geldart and Taylor<sup>15</sup> have argued that it does not decrease monotonically but instead must possess a peak for  $k \leq 2$  if one assumes that Eq. (1, 2) is correct. As Fig. 2 shows, our treatment does indeed predict such a peak in significant contrast to STLS and Hubbard. In summary, there is evidence that our theoretical expression for G(k), Eq. (4.15), and the values computed from it, Table I, are reliable for small and large values of k and correct in exhibiting a peak for values of k less than 2.

The natural extension of these calculations is the evaluation of  $G(\vec{k}, \omega)$ , that is the calculation of the quantity given in Eq. (3.5) for nonvanishing  $\omega$ ,



FIG. 2.  $G(k)/k^2$  versus  $k/k_F$ . Curve 1 is the results of the present paper; curve 2 the STLS results. Note the different behavior for  $k \leq 2$ .

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which can be used in a calculation of the pair correlation function  $g(\vec{r})$ .

The good features of G(k, 0) presented in this paper raise the hope that calculations of  $G(\vec{k}, \omega)$ and of  $g(\vec{r})$  based on the same principles will eliminate the unphysical features of previous calculations, as discussed in the Introduction.

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# APPENDIX A: DETERMINATION OF $A_{\mathfrak{q},\sigma}$

In Eq. (3.2) we write

$$H = H_0 + H_1$$

and

$$\begin{aligned} a_{\vec{a}_{1}\sigma_{1}}^{\dagger}(t)a_{\vec{k}'*\vec{s},\sigma_{1}}^{\dagger}(t)a_{\vec{s},\sigma_{1}}(t)a_{\vec{a}_{1}'\vec{k}+\vec{k}',\sigma_{1}}(t) \\ &-a_{\vec{a}_{1}-\vec{k}',\sigma_{1}}^{\dagger}(t)a_{\vec{k}'+\vec{s},\sigma_{1}}^{\dagger}(t)a_{\vec{s},\sigma_{1}}(t)a_{\vec{a}_{1}+\vec{k},\sigma_{1}}(t) = \mathfrak{C}(t), \end{aligned}$$
(A1)

$$a_{\vec{k}+\vec{q}_2,\sigma_2}^{\dagger}(0)a_{\vec{q}_2,\sigma_2}(0) = \mathfrak{B}(0).$$
 (A2)

After having carried out all the commutations involved, and using the usual approximations of the type

$$\langle a_1^{\dagger} a_2^{\dagger} a_3 a_4 \rangle = \langle a_1^{\dagger} a_4 \rangle \langle a_2^{\dagger} a_3 \rangle - \langle a_1^{\dagger} a_3 \rangle \langle a_2^{\dagger} a_4 \rangle \tag{A3}$$

and the equivalent for the average of a product of six operators, one finds

 $\lim_{t \to 0} \sum_{\mathbf{\tilde{q}}_{2}\sigma_{2}, \mathbf{\tilde{s}}_{1}\mathbf{\tilde{k}}'} v_{\mathbf{\tilde{k}}'} \langle [[\mathbf{a}(t), H_{0}], \mathbf{B}(\mathbf{0})] \rangle = \sum_{\mathbf{\tilde{q}}_{2}, \sigma_{2}} (n_{\mathbf{\tilde{k}}+\mathbf{\tilde{q}}_{2}, \sigma_{2}} - n_{\mathbf{\tilde{q}}_{2}, \sigma_{2}}) \{ \sum_{\mathbf{\tilde{k}}'} v_{\mathbf{\tilde{k}}'} \omega(\mathbf{\tilde{q}}_{2}, \mathbf{\tilde{k}}) (n_{\mathbf{\tilde{q}}_{1}+\mathbf{\tilde{k}}, \sigma_{2}} - n_{\mathbf{\tilde{q}}_{1}+\mathbf{\tilde{k}}, \sigma_{2}}) \delta_{\mathbf{\tilde{q}}_{1}\mathbf{\tilde{q}}_{2}} \delta_{\sigma_{1}\sigma_{2}} + v_{\mathbf{\tilde{k}}} \omega(\mathbf{\tilde{q}}_{2}, \mathbf{\tilde{k}}) (n_{\mathbf{\tilde{q}}_{1}+\mathbf{\tilde{k}}, \sigma_{1}} - n_{\mathbf{\tilde{q}}_{1}+\mathbf{\tilde{k}}, \sigma_{1}}) \delta_{\mathbf{\tilde{q}}_{1}\mathbf{\tilde{q}}_{2}} \delta_{\sigma_{1}\sigma_{2}}$  (A4)

and

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$$\begin{split} \lim_{t \to 0} & \sum_{\vec{\mathfrak{q}}_{2} \sigma_{2}, \vec{\mathfrak{s}} \vec{k}} v_{\vec{\mathfrak{k}}'} \langle [[\alpha(t), H_{1}] \otimes (0)] \rangle = 2 \sum_{\vec{\mathfrak{q}}_{2}} \left( (n_{\vec{\mathfrak{k}} + \vec{\mathfrak{q}}_{2}} - n_{\vec{\mathfrak{q}}_{2}}) \{ \sum_{\vec{\mathfrak{g}}_{1} \vec{k}'} v_{\vec{\mathfrak{k}}}^{2} (n_{\vec{\mathfrak{k}}' + \vec{\mathfrak{s}}}^{2} - n_{\vec{\mathfrak{q}}_{2}}^{2}) \{ \sum_{\vec{\mathfrak{g}}_{1} \vec{k}'} v_{\vec{\mathfrak{k}}}^{2} (n_{\vec{\mathfrak{k}}' + \vec{\mathfrak{s}}}^{2} - n_{\vec{\mathfrak{q}}_{2}}^{2}) \{ \sum_{\vec{\mathfrak{g}}_{1} \vec{k}'} v_{\vec{\mathfrak{k}}'}^{2} (n_{\vec{\mathfrak{k}}' + \vec{\mathfrak{s}}}^{2} - n_{\vec{\mathfrak{q}}_{2} + \vec{k}' + \vec{\mathfrak{s}}}^{2} - n_{\vec{\mathfrak{q}}_{2} + \vec{k}' + \vec{\mathfrak{s}}}^{2} - n_{\vec{\mathfrak{q}}_{2} + \vec{k}' + \vec{\mathfrak{s}}}^{2} (n_{\vec{\mathfrak{q}}_{2} + \vec{k}' + \vec{\mathfrak{s}}}^{2} - n_{\vec{\mathfrak{q}}_{2} + \vec{k}' + \vec{\mathfrak{s}}}^{2}) \} \delta_{\vec{\mathfrak{q}}_{1} \vec{\mathfrak{q}}_{2}}^{2} \\ & - \sum_{\vec{\mathfrak{s}}} \{ v_{\vec{\mathfrak{q}}_{1} - \vec{\mathfrak{q}}_{2}}^{2} [n_{\vec{\mathfrak{s}} + \vec{\mathfrak{q}}_{1} - \vec{\mathfrak{q}}_{2} + \vec{\mathfrak{s}}' + \vec{\mathfrak{s}}}^{2} (1 - n_{\vec{\mathfrak{q}}_{2} + \vec{\mathfrak{s}}' + \vec{\mathfrak{s}}}^{2} - n_{\vec{\mathfrak{q}}_{2} + \vec{\mathfrak{s}}' + \vec{\mathfrak{s}}}^{2} - n_{\vec{\mathfrak{q}}_{2} + \vec{\mathfrak{s}}' + \vec{\mathfrak{s}}}^{2} (n_{\vec{\mathfrak{q}}_{2} + \vec{\mathfrak{s}}' + \vec{\mathfrak{s}}' + \vec{\mathfrak{s}}^{2} - \vec{\mathfrak{q}}_{1}^{2}) \} \delta_{\vec{\mathfrak{q}}_{1} \vec{\mathfrak{q}}_{2}}^{2} \\ & - \sum_{\vec{\mathfrak{s}}} \{ v_{\vec{\mathfrak{q}}_{1} - \vec{\mathfrak{q}}_{2} [n_{\vec{\mathfrak{s}} + \vec{\mathfrak{q}}_{1} - \vec{\mathfrak{q}}_{2} + \vec{\mathfrak{s}}' + n_{\vec{\mathfrak{q}}_{2} + \vec{\mathfrak{s}}' - \vec{\mathfrak{q}}_{1}^{2} + \vec{\mathfrak{s}}' + n_{\vec{\mathfrak{q}}_{2} + \vec{\mathfrak{s}}' + \vec{\mathfrak{s}}'} + n_{\vec{\mathfrak{q}}_{2} + \vec{\mathfrak{s}}' + \vec{\mathfrak{s}}' + n_{\vec{\mathfrak{q}}_{2} + \vec{\mathfrak{s}}' + \vec{\mathfrak{s}}' + n_{\vec{\mathfrak{q}}_{2} + \vec{\mathfrak{s}}' + \vec{\mathfrak{s}}'} + n_{\vec{\mathfrak{q}}_{2} + \vec{\mathfrak{s}}' + \vec{\mathfrak{s}}' + n_{\vec{\mathfrak{q}}_{1} + \vec{\mathfrak{s}}' + \vec{\mathfrak{s}}'} + n_{\vec{\mathfrak{q}}_{1} + \vec{\mathfrak{s}}'} + n_{\vec{\mathfrak{q}}_{1} + \vec{\mathfrak{s}}' + n_{\vec{\mathfrak{q}}} + \vec{\mathfrak{s}}'} + n_{\vec{\mathfrak{q}}_{1} + \vec{\mathfrak{s}}' + n_{\vec{\mathfrak{s}}'} + n_{\vec{\mathfrak{s}}''} + n_{\vec{\mathfrak$$

Similarly for Eq. (3.3)

$$\lim_{t \to 0} \sum_{\vec{\mathfrak{q}}_1, \sigma_1; \vec{\mathfrak{q}}_2, \sigma_2} \langle [[a_{\vec{\mathfrak{q}}_1, \sigma_1}^{\intercal}(t) a_{\vec{k} + \vec{\mathfrak{q}}_1, \sigma_1}(t), H], a_{\vec{k} + \vec{\mathfrak{q}}_2, \sigma_2}^{\dagger}(0) a_{\vec{\mathfrak{q}}_2, \sigma_2}(0)] \rangle = -\sum_{\vec{\mathfrak{q}}_2, \sigma_2} \omega(\vec{\mathfrak{q}}_2, \vec{k}) (n_{\vec{\mathfrak{q}}_2 + \vec{k}, \sigma_2} - n_{\vec{\mathfrak{q}}_2, \sigma_2}) .$$
(A6)

In arriving at the result (3.4) we have discarded the entire term (A5) involving  $H_1$ . This amounts to neglecting the Coulomb interaction in higher order; however, it is included in some order in  $F_{\vec{\mathfrak{q}}_1,\sigma_1;\vec{\mathfrak{q}}_2,\sigma_2}^{(1)}(\vec{k},\omega)$ .

### APPENDIX B:

# **CALCULATION OF** $\lim G(k)/k^2$ as $k \to 0$

Equations (4.15), (4.10), and (4.9) lead to

$$\frac{G(k)}{k^2} = \frac{3}{8} \frac{1}{\pi^2} \left\{ \frac{1}{k^2} \int d^3 \tilde{q}_1 \int d^3 \tilde{q}_2 \left( \frac{\left[ (\tilde{q}_1 + \tilde{q}_2) \cdot \vec{k} \right]^2}{|\tilde{q}_1 + \tilde{q}_2|^2} + \frac{\left[ (\tilde{q}_1 - \tilde{q}_2) \cdot \vec{k} \right]^2}{|\tilde{q}_1 - \tilde{q}_2|^2} \right) \right\}$$

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$$\times \frac{\theta_{\langle (q_1 - \frac{k}{2})\theta_{\langle (q_2 - \frac{k}{2})\theta_{\rangle}(q_1 + \frac{k}{2})\theta_{\rangle}(q_2 + \frac{k}{2})}{(\bar{q}_1 \cdot \bar{k})(\bar{q}_2 \cdot \bar{k})} / 4 \left[ \frac{1}{2} + \frac{1}{2k} \left( 1 - \frac{4}{k^2} \right) \ln \left| \frac{k+2}{k-2} \right| \right]; \tag{B1}$$

in the limit  $k \rightarrow 0$  the denominator goes to 4, so that using (4.10) we may write

$$\lim_{k \to 0} \frac{G(k)}{k^2} = \frac{3}{8} \frac{1}{k^2} \int dq_1 \int dq_2 \int_0^1 dx_1 \int_0^1 dx_2 \left( \frac{(q_1x_1 + q_2x_2)^2}{[R_{q_1q_2}^+(x_1x_2)]^{1/2}} + \frac{(q_1x_1 - q_2x_2)^2}{[R_{q_1q_2}^-(x_1x_2)]^{1/2}} \right) \frac{q_1q_2}{x_1x_2} ,$$
(B2)

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where the limit of integration for  $q_1$  and  $q_2$  are specified by the second relation of (4.12)

$$-\frac{1}{2}kx + \left[1 + \frac{1}{4}k^2(x^2 - 1)\right]^{1/2} < q < \frac{1}{2}kx + \left[1 + \frac{1}{4}k^2(x^2 - 1)\right]^{1/2}.$$

As  $k \rightarrow 0$  we may neglect the second-order terms in k in the limits of integration and write

$$1 - \frac{1}{2}kx < q < 1 + \frac{1}{2}kx .$$

Using now the mean value theorem and the fact that we are taking the limit we may write

$$\lim_{\substack{1-\frac{kx}{2}\\\frac{1-\frac{kx}{2}}{2}}} f(q) dq = kxf(1) \text{ as } k \to 0;$$
(B4)

when applied in (B2) we obtain

$$\lim_{k \to 0} \frac{G(k)}{k^2} = \frac{3}{8} \times \frac{1}{2} \int_0^1 dx_1 \int_0^1 dx_2 (|x_1 + x_2| + |x_1 - x_2|)$$

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as 
$$[R_{1,1}(x_1, x_2)]^{1/2} = 2[(x_1 \pm x_2)^2]^{1/2}$$
. (B5)

A straightforward integration of (B5) leads directly to

 $\lim G(k)/k^2 = \frac{1}{4} .$ k → 0

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(B3)