

## Magnetic susceptibility of an electron gas in the random-phase approximation\*

B. Sriram Shastry †

Tata Institute of Fundamental Research, Homi Bhabha Road, Bombay 400005, India

(Received 2 February 1977)

The equivalence of several recent results on the spin susceptibility of the electron gas to the calculation of Brueckner and Sawada using the random-phase approximation (RPA) is reported. An error is pointed out in the exact high-density expansion of this quantity and a formula presented which is exact in the high-density limit and also accurately describes the RPA result at metallic densities.

### I. INTRODUCTION

The magnetic (spin) susceptibility of paramagnetic metals has continued to receive much attention,<sup>1-5</sup> both from theoretical and experimental workers. Recent accurate experiments on the magnitude<sup>2,3</sup> and volume dependence<sup>3</sup> of the susceptibility of the alkali metals provide a fresh impetus to the search for a comprehensive theory for this quantity. A detailed comparison of theory and experiment should contribute substantially to our understanding of the role of electron-electron interactions in metals. (The relative insensitivity of the susceptibility to the complication of electron-phonon interactions<sup>6</sup> makes the comparison more unambiguous.) Any satisfactory theory for the susceptibility must take into account two distinct aspects of the problem, namely, the solid-state (i.e., band-structure) effects and the many-body effects. A frontal attack on the problem therefore involves the calculation of many-body effects in the Bloch basis, a formidable task indeed. A promising first-principles approach due to Kohn and Sham<sup>7</sup> seeks to circumvent this by decoupling the two aspects. This method requires independent calculations of the band structure and of the susceptibility of the (uniform) electron gas<sup>8</sup> which is a somewhat simpler proposition. These calculations are finally synthesized according to a given prescription to yield the metallic susceptibility. In practice, however, their final result has not been very satisfactory and no agreement between theory and experiment seems possible. (The discrepancy for a simple metal like sodium<sup>4</sup> is much less than that for a complicated metal such as  $\alpha$ -cerium.<sup>9</sup>) Vosko and Perdew<sup>5</sup> have recently pointed out some weaknesses in the assumptions made by Kohn and Sham, and have proposed a new scheme for the susceptibility which avoids these.

Vosko and co-workers<sup>4</sup> have pointed that many recent calculations of the electron-gas susceptibility have begun to agree with each other. The calculations of Dupree and Geldart<sup>10</sup> (DG), von Barth and Hedin<sup>11</sup> (vBH), Hamann and Overhauser<sup>12</sup>

(HO), and Vasishta and Singwi<sup>13</sup> are all performed in different formalisms, and yet the final results, intriguingly enough, are the same (to within a few percent). This common result has been used by Vosko *et al.* to calculate magnitude<sup>4</sup> and the volume dependence<sup>14</sup> of the susceptibility for the alkali metals. The good overall agreement with experiments has vindicated the electron-gas susceptibility used by them, at least for  $r_s < 4$  [in terms of the electron density  $n$  and Bohr radius  $a_0$ ;  $r_s = (3/4\pi n)^{1/3} a_0$ ]. The agreement for alkali metals is very promising for the general scheme of Vosko and Perdew as well, although application of their theory to more complicated metals should present a more difficult challenge.

In this work, we examine the above-mentioned electron-gas susceptibility in detail. Since some of the authors (DG, vBH, HO) use perturbation theory in one form or another, we look for possible formal equivalences among themselves. In addition, we look for connections, if any, with the random-phase approximation (RPA) of Brueckner and Sawada<sup>15</sup> (BS). The interest in establishing this contact lies in the fact that the BS calculations is one of the very few exact results in this area. They show rigorously that at high densities, the susceptibility cannot be expanded in a power series in  $r_s$  alone, and that the long-range Coulomb interaction gives rise to  $\ln r_s$  terms just as in the ground state energy.<sup>16</sup> Their result can be conveniently expressed as

$$\chi_{BS} = \chi_P [1 - \lambda + \frac{1}{2}\lambda^2(1.534 - \ln \lambda) + O(\lambda^3)]^{-1}, \quad (1.1)$$

where

$$\lambda = \frac{\alpha r_s}{\pi}, \quad \alpha = (4/9\pi)^{1/3} \approx 0.521, \quad (1.2)$$

and  $\chi_P$  is the noninteracting Pauli susceptibility [see Eq. (2.12)]. It is to be understood in what follows that the symbol  $O(r_s^2)$  includes terms like  $(\log r_s)r_s^2$ . We must clarify at the outset that by the term RPA, we refer to the full formal expressions (obtained by summing the ring diagrams) rather than to just the high-density expansions, which are

of course latent in the former. (RPA in this sense was first used by Hubbard<sup>17</sup> to compute the ground-state energy and seems to have been first suggested by Herring<sup>18</sup> in the context of the susceptibility.)

The main difficulty in examining these relationships is that the techniques and approximations used by the above authors are very different in detail, a fact which obscures the correspondences, if any. The two main methods used to calculate the susceptibility are (a) the linear-response theory where the susceptibility is expressed in terms of Green's functions, and (b) by calculating the ground-state energy of the system as a function of the magnetization  $M$  and using the relation<sup>19</sup>

$$\chi^{-1} \propto \left. \frac{d^2 E(M)}{dM^2} \right|_{M=0}$$

There is also a third method (c) which is very closely related to method (b) where the formal expression for the ground-state energy is used to derive the Landau-interaction function from which the susceptibility may be obtained by using the Landau-theory results.<sup>20</sup> Method (a) has been used by DG and HO, and method (b) by vBH and BS. Method (c) has been pursued in detail by Herring<sup>21</sup> and Rice.<sup>22</sup> We have attacked the problem by calculating the susceptibility in a careful and complete manner by both method (a) and method (b) from the common starting point of the RPA self-energy. The approximations made are carefully kept track of, and the final results explicitly displayed to facilitate various comparisons.

The plan of the paper is as follows. Section II contains the calculation by method (a). We have developed what appears to be the simplest possible formalism within this framework. Our method requires the knowledge of only the single-particle Green's function, which after all is the simplest object that one studies in many-body theory. We express the susceptibility exactly, in terms of the magnetic field derivative of the self-energy and use the well-known RPA expression for this quantity<sup>23</sup> to derive RPA integral equations. These are tackled by methods familiar from a many body approach to Landau's Fermi-liquid theory.<sup>24</sup>

In Sec. III we obtain the susceptibility from the RPA ground-state energy. We establish contact with the BS calculation by expanding the expressions in the high-density limit. We carefully extract the high-density expansion and correct an error in the BS result [Eq. (1.1)], thus establishing the exact high-density susceptibility.

We must mention that the RPA expressions for effective-mass ( $m^*$ ) compressibility  $\kappa$  and susceptibility were first given by Rice<sup>22</sup> and computed by Lam<sup>25</sup> for  $r_s < 6$ . Nevertheless we present in Sec.

IV our somewhat more-extensive computations for  $m^*$ ,  $\kappa$ , and  $\chi$  in RPA and compare with their high-density expansions (latent in RPA) and also with other more-recent calculations, which does not seem to have been done before.<sup>26</sup> One of the useful byproducts is an empirical formula for the susceptibility which is exact to  $O(r_s^{-2})$  and accurately describes the RPA values at metallic densities.

In Sec. V, we point out the formal relationship between the work of most of the authors mentioned above and the RPA of Brueckner and Sawada. We comment on the important question of the range of validity of RPA in light of our work and discuss a possible future approach.

## II. SUSCEPTIBILITY BY THE GREEN'S-FUNCTION METHOD

The one-electron Green's function is defined in standard notation<sup>27</sup> as

$$iG_{\alpha\beta}(\vec{k}, t) = \langle 0 | T (a_{\vec{k}\alpha}(t) a_{\vec{k}\beta}^\dagger(0)) | 0 \rangle \\ = \int_{-\infty}^{+\infty} e^{-ik_0 t} G_{\alpha\beta}(k) \frac{dk_0}{2\pi}, \quad (2.1)$$

where  $k \equiv (\vec{k}, k_0)$ . In the presence of an infinitesimal magnetic field  $H = \hbar/\mu_B$  along the  $z$  axis, the up- and down-spin Green's functions are inequivalent and we denote them by  $G_\uparrow(k)$  and  $G_\downarrow(k)$ . In terms of the populations  $N_\uparrow$  and  $N_\downarrow$  of electrons with spin up and down, the magnetization is given by

$$M = \mu_B (N_\uparrow - N_\downarrow), \quad (2.2)$$

with

$$N_\sigma = -\text{Tr}_k G_\sigma(k) e^{ik_0 \eta}, \quad \eta = 0^+. \quad (2.3)$$

We have introduced the notation

$$\text{Tr}_k \equiv i \int \frac{d\vec{k}}{(2\pi)^3} \frac{dk_0}{2\pi} \quad (2.4)$$

and set the sample volume at unity for convenience. For small fields we can expand  $N_\sigma$  in powers of  $\hbar$  as

$$N_{\uparrow, \downarrow} = \frac{1}{2} N \pm \beta \hbar + O(\hbar^2), \quad (2.5)$$

where

$$\beta = -\frac{d}{d\hbar} \text{Tr}_k G_\uparrow(k) e^{ik_0 \eta} = \frac{d}{d\hbar} \text{Tr}_k G_\downarrow(k) e^{ik_0 \eta}. \quad (2.6)$$

(The limit  $\hbar \rightarrow 0$  is implicit everywhere.) The magnetization can be written

$$M = 2\mu_B \beta \hbar = 2\mu_B^2 \beta H. \quad (2.7)$$

The susceptibility is thus given by

$$\chi = 2\mu_B^2 \beta. \quad (2.8)$$

This equation is formally exact. The quantity  $\beta$  is to be obtained from the Green's function which is

given by Dyson's equation<sup>28</sup> as

$$G_{\sigma}^{-1}(k) = G_{0\sigma}^{-1}(k) - \Sigma_{\sigma}(k). \quad (2.9)$$

The self-energy  $\Sigma_{\sigma}$  is well studied in literature and can be expanded in a perturbation series in terms of the interparticle potential. The noninteracting Green's function  $G_{0\sigma}$  is given by

$$G_{0\sigma}(k) = \frac{\theta(\epsilon_F - \epsilon_{\vec{k}} + h)}{k_0 - \epsilon_{\vec{k}} + h - i\eta} + \frac{\theta(\epsilon_{\vec{k}} - h - \epsilon_F)}{k_0 - \epsilon_{\vec{k}} + h + i\eta}, \quad (2.10)$$

where  $\epsilon_{\vec{k}} = \hbar^2 k^2 / 2m$  and  $\epsilon_F = \epsilon_{k_F}$ .  $G_{0\sigma}$  is obtained from the above by changing the sign of  $h$ . Note that we have neglected the variation of the chemical potential with respect to  $h$  [which is of  $O(\hbar^2)$  (Ref. 29)] in Eq. (2.10).

For orientation, let us calculate the noninteracting susceptibility by this method. Differentiating (2.10) with respect to  $h$  we get

$$\frac{d}{dh} G_{0\sigma}(k) = -G_{0\sigma}^2(k) + (2\pi i) \delta(k_0 - \epsilon_F) \delta(\epsilon_{\vec{k}} - \epsilon_F). \quad (2.11)$$

From (2.6) and (2.8) we get the familiar Pauli susceptibility

$$\chi_P = 2\mu_B^2 n(\epsilon_F),$$

$$n(\epsilon_F) = \frac{3N}{4\epsilon_F^3} = \int \frac{d\vec{k}}{(2\pi)^3} \delta(\epsilon_{\vec{k}} - \epsilon_F). \quad (2.12)$$

It is convenient to define  $\beta$  in terms of the field derivative of the self-energy. To do this, we use (2.9) from which we get

$$\begin{aligned} \frac{d}{dh} G_{\sigma}(k) &= \lim_{h \rightarrow 0} \frac{1}{h} \{G_{\sigma}(k, h) - G_{\sigma}(k, 0)\} \\ &= - \left( 1 - \frac{d\Sigma_{\sigma}(k, h)}{dh} \right) \\ &\quad \times \lim_{h \rightarrow 0} \{G_{\sigma}(k, h) G_{\sigma}(k, 0)\}. \end{aligned} \quad (2.13)$$

The limit in (2.13) has to be taken carefully since the poles of the Green's function pinch the real  $k_0$  axis when  $k_0$  equals  $\mu$ , the chemical potential. The details are given in Appendix A and we get

$$\frac{d}{dh} G_{\sigma}(k) = -[G^2(k) + R(k)] \left( 1 - \frac{d\Sigma_{\sigma}(k)}{dh} \right), \quad (2.14)$$

where

$$R(k) = -(2\pi i) Z_{\vec{k}}^2 \delta(k_0 - \mu) \delta(E_{\vec{k}} - \mu), \quad (2.15)$$

$$Z_{\vec{k}}^{-1} = 1 - \frac{\partial \Sigma(k)}{\partial k_0}, \quad (2.16)$$

and  $E_{\vec{k}}$  is the solution of the equation

$$E_{\vec{k}} = \epsilon_{\vec{k}} + \text{Re} \Sigma(k, E_{\vec{k}}) \quad (2.17)$$

The quantity  $Z_{\vec{k}}$  is the discontinuity in occupation probability at the Fermi surface and  $E_{\vec{k}}$  is the quasiparticle energy ( $\mu = E_{k_F}$ ). We note that

$\delta(\mu - E_{\vec{k}})$  plays the role of a  $\delta$  function restricting  $\vec{k}$  to the Fermi surface and write  $R(\vec{k})$  more conveniently as

$$R(k) = -(2\pi i) Z_{\vec{k}}^2 (m^*/m) \delta(\epsilon_{\vec{k}} - \epsilon_F) \delta(k_0 - \mu), \quad (2.18)$$

with

$$\frac{m}{m^*} = \left. \frac{dE_{\vec{k}}}{d\epsilon_{\vec{k}}} \right|_{\vec{k}=\vec{k}_F}. \quad (2.19)$$

The susceptibility can finally be written

$$\chi = 2\mu_B^2 \text{Tr}_k [G^2(k) + R(k)] \left( 1 - \frac{d\Sigma_{\sigma}(k)}{dh} \right). \quad (2.20)$$

We now specialize to the RPA where the self-energy is given by<sup>23</sup>

$$\Sigma_{\sigma}(k) = \text{Tr}_{k'} V_{k-k'} G_{\sigma}(k'), \quad (2.21)$$

where  $V_q$  is the screened Coulomb interaction

$$V_q = v_q / \epsilon(q), \quad v_q = 4\pi e^2 / |\vec{q}|^2, \quad (2.22)$$

and the dielectric function is

$$\epsilon(q) = 1 + v_q \sum_{\sigma} \text{Tr}_k G_{\sigma}(k+q) G_{\sigma}(k). \quad (2.23)$$

These equations are a generalized form of RPA (termed the  $V_s$  approximation by Baym and Kadanoff) since one is using  $G$ 's to define  $\epsilon$  in (2.23) and also  $\Sigma$  in (2.21). Equation (2.21) together with Dyson's equation forms a self-consistent approximation. In our work we are not particularly concerned with the self-consistency and make the approximation that we can replace  $G$  by  $G_0$  at a sufficiently later stage so that we pick up much of the information contained in these equations. We differentiate (2.21) with respect to  $h$  and obtain the integral equation

$$\psi(k) = 1 + \text{Tr}_{k'} V_{k-k'} [G^2(k') + R(k')] \psi(k'), \quad (2.24)$$

where

$$\psi(k) \equiv 1 - \frac{d\Sigma_{\sigma}(k)}{dh}. \quad (2.25)$$

Note that  $\mu$ ,  $Z_{\vec{k}}$ , and  $m^*$  in  $R$  now refer to the RPA values rather than the exact ones. Similarly we differentiate (2.21) with respect to  $k_0$  and obtain another integral equation

$$\phi(k) = 1 + \text{Tr}_{k'} V_{k-k'} G^2(k') \phi(k'), \quad (2.26)$$

where

$$\phi(k) \equiv \frac{1}{Z_{\vec{k}}} = 1 - \frac{\partial \Sigma(k)}{\partial k_0}. \quad (2.27)$$

It is convenient to introduce an auxiliary integral equation

$$f_{k, k'} = V_{k-k'} + \text{Tr}_{k''} V_{k-k''} G^2(k'') f_{k'', k'}, \quad (2.28)$$

which defines the function  $f$ . It is clear that  $G^2(k')f_{k,k'}$  is the resolvent kernel of (2.26) from which we get

$$\phi(k) = 1 + \text{Tr}_{k'} f_{k,k'} G^2(k'). \quad (2.29)$$

The formal solutions for  $\psi$ ,  $\phi$ , and  $f$  are

$$\begin{aligned} \psi &= [1 - V(G^2 + R)]^{-1} \mathbf{1}, \quad \phi = (1 - VG^2)^{-1} \mathbf{1}, \\ f &= (1 - VG^2)^{-1} V. \end{aligned} \quad (2.30)$$

The solution for  $\psi$  can be written in the form

$$\psi = [1 - V(G^2 + R)]^{-1} (1 - VG^2)\phi, \quad (2.31a)$$

which simplifies to

$$\psi = (1 - fR)^{-1}\phi. \quad (2.31b)$$

This equation can be rewritten

$$\psi(k) = \phi(k) + \text{Tr}_{k'} f_{k,k'} R(k')\psi(k') \quad (2.32)$$

The  $\delta$ -function property of  $R$  reduces the above equation to an algebraic equation. Thus both  $\psi$  and  $\phi$  are determined by the function  $f$ . We can rewrite (2.32) on using (2.18) as

$$\begin{aligned} \psi(k) &= \phi(k) + \psi(k_F) \left( \frac{m^*}{m} Z_{k_F}^2 n(\epsilon_F) \right. \\ &\quad \left. \times \int f(\vec{k}, \vec{k}_F) \frac{d\Omega_{\vec{k}_F}}{4\pi} \right), \end{aligned} \quad (2.33)$$

with  $\psi(k_F) \equiv \psi(\vec{k}_F, \mu)$ . Using (2.20), (2.25), (2.27), (2.29), and (2.33) we get

$$\begin{aligned} \frac{\chi}{2\mu_B^2} &= -\text{Tr}_k \frac{\partial}{\partial k_0} G(k) + \text{Tr}_k R(k)\psi(k) \\ &\quad + \frac{m^*}{m} Z_{k_F} n(\epsilon_F) (1 - Z_{k_F}) \psi(k_F). \end{aligned} \quad (2.34)$$

The first term vanishes on integrating by parts and the remaining terms can be collected together and give

$$\chi = \chi_P \left( \frac{m}{m^*} - Z_{k_F}^2 n(\epsilon_F) \int f(\vec{k}_F, \vec{k}_F) \frac{d\Omega_{\vec{k}_F}}{4\pi} \right)^{-1}. \quad (2.35)$$

This equation is of the Landau-theory form if we identify  $-Z_{k_F}^2 f_{k,k'}$  as the exchange interaction function of Landau.<sup>20</sup> We still need to solve the integral equation (2.28) to obtain  $f$  but we can seek iterative solutions which are to the lowest order in the screened interaction (the RPA solution). To this order, it is clear that we can replace  $f$  by  $V_{\text{RPA}}$  in (2.35) and also set  $Z_k$  as unity. [ $V_{\text{RPA}}$  now stands for  $v/\epsilon_{\text{RPA}}$ , where (2.23) is evaluated with  $G_0$ 's rather than  $G$ 's.] After scaling the momenta by  $k_F$  and frequencies by  $2\epsilon_F$ , the expression can be written in high-density units as

$$\chi_{\text{RPA}} = \chi_P \left( \frac{m}{m^*} - \lambda \int_0^2 \frac{dq}{q} \frac{1}{\epsilon_{\text{RPA}}(q, 0)} \right)^{-1}. \quad (2.36)$$

The calculation of  $m/m^*$  in RPA can be done by

using Eqs. (2.19), (2.17), and (2.21). The calculation is straightforward<sup>22,30</sup> and gives

$$\begin{aligned} \frac{m}{m^*} &= 1 - \lambda + \lambda \int_0^2 \frac{dq}{q} \frac{1}{\epsilon_{\text{RPA}}(q, 0)} \\ &\quad - \frac{\lambda}{2\pi} \int_0^\infty \int_0^\infty dq du \left( \frac{1}{\epsilon_{\text{RPA}}(q, iqu)} - 1 \right) F(q, u), \end{aligned} \quad (2.37)$$

with

$$\begin{aligned} F(q, u) &= \ln \left( \frac{u^2 + (1 + \frac{1}{2}q)^2}{u^2 + (1 - \frac{1}{2}q)^2} \right) \\ &\quad - \frac{2+q}{u^2 + (1 + \frac{1}{2}q)^2} + \frac{2-q}{u^2 + (1 - \frac{1}{2}q)^2}. \end{aligned} \quad (2.38)$$

This gives the final expression for the RPA susceptibility as

$$\begin{aligned} \chi_{\text{RPA}} &= \chi_P \left[ 1 - \lambda - \frac{\lambda}{2\pi} \int_0^\infty \int_0^\infty dq du \left( \frac{1}{\epsilon_{\text{RPA}}(q, iqu)} - 1 \right) \right. \\ &\quad \left. \times F(q, u) \right]^{-1}. \end{aligned} \quad (2.39)$$

The last term on the right-hand side represents the correlation correction to the susceptibility and is evaluated in Sec. IV. Explicit formulas for  $\epsilon_{\text{RPA}}$  are given in Appendix B.

### III. SUSCEPTIBILITY FROM THE GROUND-STATE ENERGY AND THE EXACT HIGH-DENSITY EXPANSION

We constrain the  $N$ -electron system to a magnetized state with a polarization  $p$  given by

$$p = (N_\uparrow - N_\downarrow)/N. \quad (3.1)$$

The Fermi momenta of the spin-up and -down electrons are given by

$$k_{F\pm} = k_F (1 \pm p)^{1/3}. \quad (3.2)$$

The ground-state energy  $E(p)$  in this constrained situation can be used to obtain the susceptibility through the well known relation<sup>19</sup>

$$\chi = \chi_P \left( \frac{d^2 E_0(p)}{dp^2} \right)_{p=0} \left/ \left( \frac{d^2 E(p)}{dp^2} \right)_{p=0} \right., \quad (3.3)$$

where  $E_0(p)$  is the non interacting case energy. Thus an approximation for the ground state energy automatically generates one for the susceptibility. The interaction energy ( $E_{\text{int}} = E - E_0$ ) is well known<sup>31</sup> to be expressible in terms of the self-energy and the Green's function as

$$\begin{aligned} E_{\text{int}} &= -\frac{1}{2} \int_0^1 \frac{d\lambda'}{\lambda'} \text{Tr}_k e^{ik_0\eta} \\ &\quad \times [\Sigma_\uparrow^\lambda(k) G_\uparrow^\lambda(k) + \Sigma_\downarrow^\lambda(k) G_\downarrow^\lambda(k)], \end{aligned} \quad (3.4)$$

where the coupling constant is taken as  $\lambda'e^2$  in place of  $e^2$ . Therefore as in Sec. II, an approxima-

tion for the self-energy is sufficient to calculate the susceptibility.

We have already noted the RPA expression for the self-energy in Eq. (2.21). We can directly set the  $G$ 's in Eq. (2.21) and (2.23) as  $G_0$ 's, i.e., the noninteracting Green's function [explicit expressions for  $G_0$  in the polarized case is given in Appendix B, Eq. (B3)]. This self-energy can be substituted in (3.4) and  $G^N$  replaced by  $G_0$  to get the interaction energy to *lowest order in the screened-Coulomb interaction*. The coupling-constant integration is trivial and gives the correlation energy (defined as  $E - E_{\text{HF}}$ , where HF stands for Hartree-Fock) in RPA as

$$E_{\text{corr}}(p) = -\frac{1}{2} \text{Tr}_k [\ln \epsilon_{\text{RPA}}(k) + 1 - \epsilon_{\text{RPA}}(k)]. \quad (3.5)$$

The momenta are scaled by  $k_F$  and frequencies by  $2\epsilon_F$  to give the correlation energy per particle (in rydbergs) as

$$\epsilon_{\text{corr}}(p) = \frac{3}{2\pi^3} \frac{1}{\lambda^2} \int_0^\infty \int_0^\infty k^3 dk du [\ln \epsilon_{\text{RPA}}(k, iku) + 1 - \epsilon_{\text{RPA}}(k, iku)]. \quad (3.6)$$

We have used the analyticity of  $\epsilon_{\text{RPA}}$  as a function of frequency in the first and third quadrants<sup>30</sup> to transform the integration to the imaginary axis. This equation, together with Eqs. (B1) and (B5) is identical to Eq. (5) of BS. Following BS, we define

$$\alpha_c \equiv 2 \left. \frac{d^2}{dp^2} \epsilon_{\text{corr}}(p) \right|_{p=0}. \quad (3.7)$$

We can use the well-known expressions<sup>15</sup> for  $E_0(p)$  and  $E_{\text{exchange}}(p)$  to arrive at the expression for the susceptibility

$$\chi = \chi_P [1 - \lambda + \frac{3}{4}\pi^2 \lambda^2 \alpha_c]^{-1}. \quad (3.8)$$

It is worth mentioning that this equation would be exact if  $\alpha_c$  were exactly known.

To proceed further, we substitute for  $\epsilon_{\text{RPA}}$  from (B9) and use (3.6) in (3.7) to get the RPA expression for  $\alpha_c$  as

$$\alpha_c = \frac{2}{3\pi^4} \int_0^\infty \int_0^\infty dq du \frac{Q_q(u)}{q^2 + (\lambda/\pi)Q_q(u)} F(q, u). \quad (3.9)$$

This equation can be combined with (3.8) and it is readily seen that the susceptibility obtained is identical to Eq. (2.39). Thus we have established that the same expression for susceptibility results both by method (a) and (b).

As already mentioned in Sec. I, Brueckner and Sawada were primarily interested in the high-density limit. They did not obtain Eq. (3.9) (where the small  $r_s$  assumption has not been made) but rather, directly analyzed the series obtainable from Eq. (3.6) for small  $r_s$ . It is very illuminating, however, to follow an alternative procedure and to ex-

tract the high-density behavior directly from (3.9). In order to do this, we first observe that

$$F(q, u) = \frac{4q}{q^2 + (1+u^2)^2} \quad (3.10)$$

As a result  $\alpha_c$  is logarithmically divergent in the limit  $\lambda \rightarrow 0$  and has the behavior

$$\alpha_c \underset{\lambda \rightarrow 0}{\sim} a_1 + a_2 \ln \lambda + O(\lambda). \quad (3.11)$$

Thus a calculation of  $a_1$  and  $a_2$  gives the susceptibility correct to  $O(r_s^2)$ . In order to obtain the logarithmic term  $a_2$ , it suffices to cut the  $q$  integration off (at  $q=1$  for convenience), and to replace the integrand by the small- $q$  behavior. Thus we define

$$\alpha_{1n} \equiv \frac{8}{3\pi^4} \int_0^\infty du \frac{Q_0(u)}{(1+u^2)^2} \int_0^1 \frac{q dq}{q^2 + (\lambda/\pi)Q_0(u)}. \quad (3.12)$$

We can use Eq. (B13) for  $Q_0$  to get

$$\alpha_{1n} = -\frac{2}{3\pi^2} \left( \ln 4\lambda + \frac{8}{\pi} \int_0^\infty \frac{du}{(1+u^2)^2} R(u) \ln R(u) \right). \quad (3.13)$$

The second term is precisely  $\langle \ln R \rangle_{\text{av}}$  of BS which they have numerically evaluated as  $-0.534$ . Thus we get

$$\alpha_{1n} = (2/3\pi^2)(0.534 - \ln 4\lambda). \quad (3.14)$$

It is clear from (3.14) that  $a_2 = -2/3\pi^2$ . The quantity  $\alpha_{1n}$  also contains a part of the constant term  $a_1$ . In order to get the remaining contribution to  $a_1$  we must take the difference of Eqs. (3.9) and (3.14) which is finite in the limit  $\lambda \rightarrow 0$ . Thus define

$$\alpha^{(0)} \equiv \lim_{\lambda \rightarrow 0} (\alpha_c - \alpha_{1n}). \quad (3.15)$$

In terms of  $\alpha^{(0)}$ , it is clear that

$$a_1 = \alpha^{(0)} + (2/3\pi^2)(0.534 - \ln 4). \quad (3.16)$$

The expression for  $\alpha^{(0)}$  is readily obtained from (3.9) and (3.12) as

$$\alpha^{(0)} = \lim_{\lambda \rightarrow 0} \frac{2}{3\pi^2} \left( \frac{1}{\pi^2} \int_0^\infty du \int_\eta^\infty \frac{dq}{q^2} Q_q(u) F(q, u) - \frac{16}{\pi} \int_0^\infty \frac{du R(u)}{(1+u^2)^2} \int_\eta^1 \frac{dq}{q} \right). \quad (3.17)$$

This integral can be numerically evaluated (by the method discussed<sup>32</sup> in Sec. IV) and gives

$$\alpha^{(0)} \simeq (2/3\pi^2)(1.157). \quad (3.18)$$

This is very different from the value  $(2/3\pi^2)(2.386)$  obtained by BS, and led us to reexamine their lengthy and involved calculation. To reestablish contact we rewrite (3.17) in terms of  $Q_q^*$  and  $Q_q$  as

$$\alpha^{(0)} = \left( \frac{d^2}{dp^2} \right)_{p \rightarrow 0} \lim_{n \rightarrow 0} \left( -\frac{3}{\pi^5} \right) \times \int_{\eta}^{\infty} \frac{dq}{q} \int_0^{\infty} du [Q_q(u)Q_q^*(u) - \theta(1-q)Q_0(u)Q_0^*(u)]. \quad (3.19)$$

The integration over  $u$  is readily performed on using the integral representation (B6) for  $Q_q(u)$  and the result is expressible as

$$\alpha^{(0)} = \frac{1}{4} \frac{\partial^2}{\partial p^2} f((1+p)^{1/3}, y) \Big|_{p=0, y=1}, \quad (3.20)$$

where

$$f(x, y) = \left( -\frac{3}{2\pi^4} \right) \lim_{n \rightarrow 0} \int_{\eta}^{\infty} \frac{dq}{q} [h(x, y; q) - \theta(1-q)h(x, y; 0)] \quad (3.21)$$

and

$$h(x, y; q) = \frac{1}{q} \int \int \frac{d\vec{k}_1 d\vec{k}_2}{\vec{q} \cdot (\vec{k}_1 + \vec{k}_2 + \vec{q})} \times \theta(x - k_1) \theta(|\vec{k}_1 + \vec{q}| - x) \times \theta(y - k_2) \theta(|\vec{k}_2 + \vec{q}| - y). \quad (3.22)$$

We can set  $(1+p)^{1/3} = x$  in (3.20) which gives

$$\alpha^{(0)} = \frac{4}{9} \left( \frac{\partial^2}{\partial x^2} - 2 \frac{\partial}{\partial x} \right) f(x, y) \Big|_{x=1, y=1}. \quad (3.23)$$

It is clear that (3.21) and (3.23) are identical to Eqs. (A2) and (A4) of BS [since  $\alpha^{(0)} = (4/p^2) \{ \delta(p) - \delta(0) \}$  in their notation]. In order to proceed further BS assert that  $f(x, x)$  is proportional to  $x^3$ , which leads to a considerable simplification since we can then transform (3.23) into a form involving only

$$\left. \frac{\partial^2 f(x, y)}{\partial x \partial y} \right|_{x=1, y=1}.$$

[This quantity is much simpler to evaluate since the mixed derivative leads to  $\delta$  functions in (3.22) constraining both  $\vec{k}_1$  and  $\vec{k}_2$  to the Fermi surface.] This assertion is prompted by the scaling property of  $h$ :

$$h(x, x; q) = x^3 \bar{\phi}(q/x). \quad (3.24)$$

This may be substituted in (3.21) and gives

$$f(x, x) = x^3 \left( -\frac{3}{2\pi^4} \right) \lim_{\eta \rightarrow 0} \left( \bar{\phi}(0) \ln \eta + \int_{\eta/x}^{\infty} \frac{dt}{t} \bar{\phi}(t) \right). \quad (3.25)$$

The second term can be integrated in a small neighborhood of the lower limit and gives

$$f(x, x) = x^3 (-3/2\pi^4) \lim_{\eta \rightarrow 0} [\bar{\phi}(0) \ln \eta + K - \bar{\phi}(0) \ln(\eta/x)], \quad (3.26)$$

where  $K$  is independent of  $x$ . The limit is now trivial and results in

$$f(x, x) = -(3/2\pi^4) [x^3 K + x^3 \bar{\phi}(0) \ln x]. \quad (3.27)$$

Thus the assertion of BS is not correct and  $f(x, x)$  has a  $x^3 \ln x$  term in addition to the  $x^3$  term, and hence their identity equation (A5) is not applicable. The log term however enters the above equation with the well-known coefficient<sup>33</sup>

$$\bar{\phi}(0) = \frac{8}{3} \pi^2 (1 - \ln 2). \quad (3.28)$$

We can use Eq. (3.27) to derive an identity<sup>34</sup>

$$\left( \frac{\partial^2}{\partial x^2} - 2 \frac{\partial}{\partial x} + \frac{\partial^2}{\partial x \partial y} \right) f(x, y) \Big|_{x=1, y=1} = \frac{3}{2} \left( -\frac{3}{2\pi^4} \right) \bar{\phi}(0). \quad (3.29)$$

This is the same as identity (A5) of BS except for the term on the right-hand side. The first term has already been evaluated by BS as

$$\left. \frac{\partial^2}{\partial x \partial y} f(x, y) \right|_{x=1, y=1} = -\frac{3}{\pi^2} (\ln 2 + \frac{1}{2}). \quad (3.30)$$

We obtain  $\alpha^{(0)}$  from (3.23), (3.28), and (3.30) as

$$\alpha^{(0)} = (2/3\pi^2) (6 \ln 2 - 3), \quad (3.31)$$

which clearly agrees with (3.18), and together with (3.8) and (3.16) gives the exact high-density susceptibility

$$\chi_{\text{exact}} \stackrel{\equiv}{=} \chi_P [1 - \lambda + \frac{1}{2} \lambda^2 (0.306 - \ln \lambda) + O(\lambda^3)]^{-1}. \quad (3.32)$$

#### IV. NUMERICAL RESULTS

The RPA susceptibility expression (2.39) involves a double integral which was evaluated as follows. The algebraic substitutions  $x = q/(1+q)$  and  $y = u/(1+u)$  convert the area of integration into the unit square. The unit square was subdivided systematically into several small squares ( $\sim 200$ ) and the contribution from each was evaluated by a nine-point two-dimensional Gaussian quadrature formula.<sup>35</sup> The weak singularity of the integrand at  $u = 0$ ,  $q \sim 2$  was handled accurately by separating the  $x$  interval into two regions corresponding to  $q \leq 2$ , and  $q > 2$ , and by rescaling the rectangles into squares by suitable substitutions. The results are presented in Table I and compared with the high-density formula (3.32). Our computation can be accurately fitted in the metallic density range  $r_s < 6$  by the formula

$$\chi_{\text{RPA}} = \chi_P \{ 1 - \lambda + \frac{1}{2} \lambda^2 [0.309 - \ln \lambda + f(\lambda)] \}^{-1}, \quad (4.1a)$$

where

$$f(\lambda) = 1.168\lambda - 0.900\lambda^2 + 0.383\lambda^3. \quad (4.1b)$$

TABLE I. Susceptibility  $\chi/\chi_P$  for various  $r_s$  ( $\chi_P = 2.589r_s^{-1} \times 10^{-6}$  cgs volume units).

$r_s$	RPA Eq. (2.39)	High density Eq. (3.32)	$r_s$	RPA Eq. (2.39)	High density Eq. (3.32)
0.5	1.079	1.079	3.5	1.566	1.777
1	1.155	1.158	4	1.658	2.024
1.5	1.233	1.244	4.5	1.756	2.379
2	1.311	1.341	5	1.859	2.902
2.5	1.393	1.455	5.5	1.969	3.948
3	1.477	1.596	6	2.086	6.32

This formula was obtained by a least-squares fit after removing the known logarithmic term, and incidentally provides an independent check on the exact result (3.32). The formula has the virtue of being formally exact to  $O(r_s^2)$  and should be useful in calculations based on the theory of Vosko and Perdew.<sup>4,5</sup>

In Fig. 1, we compare the exact result for the inverse susceptibility  $\chi_P/\chi$  [Eq. (3.32)] with the Brueckner-Sawada result [Eq. (1.1)] to give an idea of the numerical difference made by our correction of their result. For comparison we have also plotted the RPA susceptibility inverse obtained by our computation of Eq. (2.39). It is readily seen from the figure that the exact result (3.32) and the RPA are nearly identical for  $r_s \lesssim 2.5$ , which is, of course, as it should be. We have also included the Hartree-Fock result ( $1 - \lambda$ ) for comparison since it is exact to  $O(r_s)$ . By a coincidence the RPA and the BS susceptibilities blow up at nearly the same value of  $r_s$  ( $\sim 18$ ), and the Hartree-Fock as well as our exact result also [Eq. (3.32)] blow up for  $r_s \sim 6$ .

In Table II we present the RPA effective mass  $m^*$  [see Eq. (2.37)] compared with the results of other theories and also with the high density expansion of

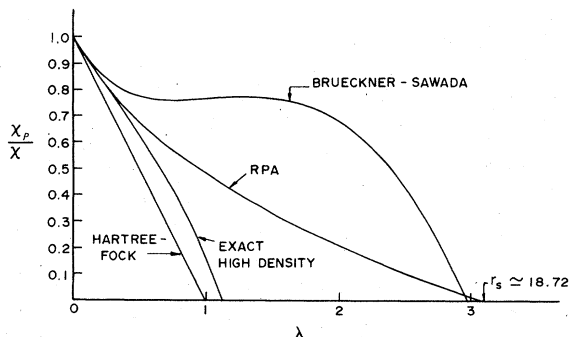


FIG. 1. Inverse susceptibility for various values of  $\lambda (= r_s/6.029)$ . The curve marked Brueckner-Sawada is from Ref. 15 [see Eq. (1.1.)]. The curve marked "exact high density" is a result of this work where we have corrected one of the two terms obtained by BS [see Sec. III, Eq. (3.32)]. The RPA curve is obtained from a computation of Eq. (2.39).

this quantity given by<sup>36</sup>

$$m/m^*_{\lambda \rightarrow 0} = 1 - \lambda(1 + \frac{1}{2} \ln \lambda) + O(\lambda^2). \quad (4.2)$$

In Table III we present the RPA compressibility given by<sup>22</sup>

$$\frac{\kappa_F}{\kappa} = \frac{\chi_P}{\chi_{RPA}} - \frac{\lambda^2}{\pi} \int_0^\infty \int_0^\infty q dq du \left[ \frac{1}{q^2 \epsilon_{RPA}(q, iqu)} \times \ln \left( \frac{u^2 + (1 + \frac{1}{2}q)^2}{u^2 + (1 - \frac{1}{2}q)^2} \right) \right]^2. \quad (4.3)$$

We compare the result with those of other theoretical calculations and also with the high-density expansion<sup>37</sup> (obtained from the Gell-Mann-Brueckner calculation<sup>16</sup>)

$$\frac{\kappa_F}{\kappa}_{\lambda \rightarrow 0} = 1 - \lambda - (1 - \ln 2)\lambda^2 + O(\lambda^3). \quad (4.4)$$

The remarkable point to note in Tables II and III is that although the high-density results (latent in RPA) are not close to those of more-sophisticated theories at metallic densities, the RPA results are very close indeed, and have the added virtue of being very exact at high densities. An analogous behavior of the correlation energy was first pointed out by Hubbard.<sup>17</sup>

## V. DISCUSSION AND CONCLUSION

One of the main results of this work is Eq. (3.32), the exact high-density expansion of the susceptibility to  $O(r_s^2)$ . It is clear from Fig. 1 that the change

TABLE II. Effective mass  $m^*/m$  in various theories.

$r_s$	RPA (present paper)	Exact high density Eq. (4.2)	Nozières-Pines (Ref. 22)	Hubbard (Ref. 40)
1	0.968	1.017		0.963
2	0.992	1.174	1.02	0.985
3	1.026	1.479	1.05	1.019
4	1.065	2.115	1.1	1.057
5	1.106			1.099
6	1.149			1.144

TABLE III. Compressibility ratio  $\kappa_F/\kappa$  in various theories.

$r_s$	RPA (present paper)	Exact high density Eq. (4.4)	Hubbard (Ref. 40)	Wigner (Ref. 22)	Nozières- Pines (Ref. 22)	Vasishta- Singwi (Ref. 42)
1	0.827	0.827	0.831	0.83	0.83	0.839
2	0.642	0.634	0.665	0.66	0.65	0.653
3	0.446	0.426	0.472	0.46	0.46	0.454
4	0.242	0.201	0.282	0.26	0.27	0.246
5	0.031	-0.04	0.086			0.032
6	-0.187		-0.116			-0.186

in the magnitude of the  $O(r_s^2)$  term from 1.534 to 0.306 makes a substantial difference in the behavior of the susceptibility. Our susceptibility is larger than the BS result for all densities. The RPA susceptibility is almost identical to the high-density result for  $r_s \approx 2.5$  and is smaller for  $r_s > 2.5$ . We note that our high-density susceptibility diverges at  $r_s \approx 6.6$  and the RPA at  $r_s \approx 18.72$ . It seems difficult, however, to identify this with a physical instability of the electron gas towards a magnetically ordered phase in view of the fact that the compressibility already blows up for a smaller value of  $r_s$  ( $\sim 5.1$ ).

Turning to the formal problem, we summarize the main steps involved in obtaining the susceptibility by the two methods (a) and (b) used in Secs. II and III. We have deliberately chosen a common starting point for both calculations, namely, the self-energy expression Equation (2.21), in order to give the reader a clear idea of the relative effort involved in the two methods. In method (a) we first set up integral equations for certain derivatives of the self-energy and obtain a formal solution (2.35) for the *inverse susceptibility*  $\chi_p/\chi$  in terms of an "interaction function" which obeys another integral equation. The RPA susceptibility is then obtained on approximating the formal solution by throwing out terms which are of second and higher order in the RPA screened-Coulomb interaction. In method (b), however, we directly approximate the self-energy by the RPA expression (i.e., replace  $G$ 's by  $G_0$ 's) and differentiate this with respect to the polarization to get the RPA expression for  $\chi_p/\chi$ . Thus, method (b) gives the same results as method (a) with considerably less effort.

Among the calculations mentioned in Sec. I, Dupree and Geldart use method (a). They define a triplet vertex part  $\Lambda_p^1(k)$  that obeys an integral equation in which the limit  $\vec{k} \rightarrow 0, k_0 \rightarrow 0; k_0/|\vec{k}| \rightarrow 0$  is identical to ours [Eq. (2.24)] (which could be the consequence of a possible Ward identity). The details of their calculation are unfortunately not given, but one may infer that their approximations amount to just the RPA. We mention in the passing

that the dynamically screened interaction in Eq. (2.24) is often approximated by<sup>12, 37-39</sup> a statically screened (Yukawa) interaction. The integral equation then reduces to an algebraic one, which is readily solved<sup>12, 37, 38</sup> and has the same form as (2.36) (with a different expression for  $m^*/m$ ), but does not give the correct high-density behavior (3.32). Thus the frequency dependence of  $\epsilon_{\text{RPA}}$  is crucial in obtaining the correct high-density limit.

The calculation of Hamann and Overhauser is also based on method (a). They have avoided the use of field-theoretic methods and instead use a canonical transformation to derive an integral equation. Their equation (25) in the limit  $\vec{q} \rightarrow 0$  is equivalent to our equation (2.24) with the approximations after (2.35) already made. They have not used the simplification resulting from a transformation of the frequency integral to the imaginary axis, but directly compute the expressions. Thus they have also rediscovered the RPA in another form.

We have already made explicit contact with the Brueckner-Sawada calculation in Sec. II. The calculation of von Barth and Hedin is identical, *in principle*, to our calculation since their "two-bubble" approximation for the proper polarization part is nothing but the RPA. They evaluate the correlation energy for various values of the polarization and differentiate this quantity numerically rather than analytically (which should account for the small discrepancies between their values and ours). They have expressed surprise that their seemingly naive approach gives the same results as those of a much more sophisticated theory such as that of DG. It should, however, be clear from our discussion that the coincidence of results is due to the fact that both VBH and DG as well as HO have merely rediscovered the RPA by various methods.

We mentioned the method (c) (i.e., the Landau theory) briefly in Sec. I as a variant of method (b). As mentioned in Sec. IV, explicit calculation of the RPA susceptibility by this method has been given by Rice.<sup>24, 40</sup> The resulting expressions, not unexpectedly, are the same as ours.



In conclusion, it is pertinent to remark on the range of validity of RPA and possibilities of future developments of the theory, based on the facts that we have encountered so far. Our demonstration that several authors have rediscovered the RPA by various methods implies that the validity of the common result of high densities, say  $r_s \lesssim 2.5$  is assured on rigorous grounds. On the other hand, it also implies that the agreement among the authors cannot be cited as a "proof" of the essential correctness of the final result, and hence one could expect departures from the RPA at lower densities. As mentioned in Sec. I, experiments support the RPA result in the density range  $r_s \lesssim 4$ . This fact, together with the closeness of RPA results for  $m^*$ ,  $\kappa$  and correlation energy with other contemporary (nonperturbative) theories, strongly indicates that the non-RPA terms are numerically negligible in the density range  $r_s \lesssim 4$ . Thus any departure of the susceptibility from the RPA can be expected to occur only for  $r_s > 4$ , especially since the RPA compressibility diverges at  $r_s \sim 5.1$  (see Table III) signaling a breakdown of the approximation.

A possible approach to go beyond RPA is suggested by the approximations we made in Sec. II. We found that the RPA was obtained by retaining all terms which are of "first order" in the RPA screened-Coulomb interaction  $v/\epsilon_{\text{RPA}}$ . This certainly is not perturbation theory of the usual kind since  $v/\epsilon_{\text{RPA}}$  is a *function* and not a parameter. This suggests that we can think of an interesting rearrangement of terms in the perturbation theory (for instance, by regrouping Feynman diagrams) to obtain a formal development of the relevant quantities (self-energy, etc.) in terms of the function  $v/\epsilon_{\text{RPA}}$  (which would mimic the role of a coupling constant in order counting). Thus RPA would be the lowest-order theory in this sense, and a logical sequel would involve retention of all terms containing *two* RPA interactions. [Based on our discussion of the two methods (a) and (b), this should be simpler by method (b).] We have started work

$$\frac{Z_k}{k_0 - E_k^- + \alpha_k^- h + i\eta \text{sign}(E_k^- - \alpha_k^- h - \mu)} = \frac{Z_k}{k_0 - E_k^- + \alpha_k^- h + i\eta \text{sign}(E_k^- - \mu)} + i\pi Z_k \delta(k_0 - E_k^- + \alpha_k^- h) [\text{sign}(E_k^- - \mu) - \text{sign}(E_k^- - \alpha_k^- h - \mu)]. \quad (\text{A4})$$

We can multiply the first term by the pole part of (A1) and get terms which have poles on same side of the real axis, in which the limit  $h \rightarrow 0$  may be taken without difficulty. The second term of the right-hand side can be multiplied by the pole part of (4.4) and gives

$$\frac{i\pi Z_k^2}{-\alpha_k^- h} \delta(k_0 - E_k^- + \alpha_k^- h) [\text{sign}(E_k^- - \mu) - \text{sign}(E_k^- - \alpha_k^- h - \mu)]. \quad (\text{A5})$$

on such a program and hope to present the results soon.

*Note added in proof.* A brief announcement of the exact result Eq. (3.32) has appeared recently.<sup>43</sup>

#### APPENDIX A: THE LIMIT OF $\{G_{\uparrow}(k, k)G_{\uparrow}(k, 0)\}$ AS $k \rightarrow 0$

This limit is very similar to the limit  $\vec{q} \rightarrow 0, q_0 \rightarrow 0, G(k+q)G(k)$ , which is considered in detail by Nozières.<sup>24</sup> Let us recall the paramagnetic phase where we note from Dyson's equation (2.9) that  $G_{\uparrow}(k, 0)$  has a pole at  $k_0 = E_k$  which is the solution of Eq. (2.17), with residue  $Z_k$ . (The imaginary part of  $\Sigma$  is vanishingly small for  $k \sim k_F$ .) Thus the Green's function may be decomposed for  $k \sim k_F$  as

$$G_{\uparrow}(k, 0) = G_{\uparrow \text{inc}}(k, 0) + Z_k^- / [k_0 - E_k^- + i\eta \text{sign}(E_k^- - \mu)]. \quad (\text{A1})$$

where  $G_{\uparrow \text{inc}}$  is the coherent part of the Green's function which is smooth as  $k_0$  passes through  $E_k^-$ . As usual the poles have been displaced above (below) the real axis for  $E_k < \mu$  ( $E_k > \mu$ ).

In the presence of a small magnetic field we note from (2.9) that  $G_{\uparrow}^{-1}(k, h)$  has a zero for  $k_0 = E_k^- - \alpha_k^- h$ , where  $\alpha_k^- = Z_k^- [1 - d\Sigma_{\uparrow}(k, h)/dh]$ . Thus the Green's function can be decomposed as before into a pole part and an incoherent part. For  $h \rightarrow 0, k \sim k_F$ , we have

$$G_{\uparrow}(k, h) = G_{\uparrow \text{inc}}(k, h) + Z_k^- / [k_0 - E_k^- + \alpha_k^- h + i\eta \text{sign}(E_k^- - \alpha_k^- h - \mu)]. \quad (\text{A2})$$

When we multiply (A1) with (A2) and take limit  $h \rightarrow 0$ , we would merely get a factor  $G_{\uparrow}^2(k, 0)$  but for the singular terms arising from the two pole parts, when the poles are on the opposite sides of the real axis. To simplify the calculation, we use the symbolic identity

$$1/(x \mp i\eta) = p(1/x) \pm i\pi \delta(x) \quad (\text{A3})$$

in the pole term of (A2). Thus we write

The limit  $h \rightarrow 0$  can now be taken, and on using  $(d/dx) \text{sign}(x) = 2\delta(x)$ , we see that (A5) is nothing but  $R(k)$  defined in (2.15). All the remaining terms add up to give  $G^2(k)$  and hence the result (2.14).

#### APPENDIX B: SOME USEFUL PROPERTIES OF $\epsilon_{\text{RPA}}$

In this appendix we collect some well-known<sup>30, 41</sup> properties of the RPA dielectric function and de-

rive a useful expansion for small spin polarization. The propagating RPA dielectric function can be written [see Eq. (2.23) with noninteracting Green's functions]

$$\epsilon_{\text{RPA}}(q) = 1 + \frac{1}{2} [Q_{\uparrow}(q) + Q_{\downarrow}(q)], \quad (\text{B1})$$

where

$$Q_{\sigma}(q) = 2v_{\sigma} \text{Tr}_k G_{\sigma\sigma}(k+q) \dot{G}_{\sigma\sigma}(k). \quad (\text{B2})$$

The noninteracting Green's function in the spin-polarized case is given by

$$G_{0\uparrow, \downarrow}(k) = \frac{f_k^{\pm}}{k_0 - \epsilon_k^{\pm} - i\eta} + \frac{1 - f_k^{\pm}}{k_0 - \epsilon_k^{\pm} + i\eta}, \quad (\text{B3})$$

where the Fermi functions are defined as usual:

$$f_k^{\pm} = \theta(k_{F\pm} - k) = \theta(1 \pm p - k^3/k_F^3). \quad (\text{B4})$$

[We have used Eq. (3.2) to express  $k_{F\pm}$  in terms of the polarization.] The  $k_0$  integration in (B2) is straightforward and we get

$$Q_{\uparrow, \downarrow}(q, iqu) = (\lambda/\pi q^2) Q_q^{\pm}(u), \quad (\text{B5})$$

where  $Q_q^{\pm}(u)$  is the Gell-Mann-Brueckner screening function

$$Q_q^{\pm}(u) = \int d\vec{k} f_k^{\pm} (1 - f_{k+\vec{q}}^{\pm}) \frac{2(\frac{1}{2}q^2 + \vec{k} \cdot \vec{q})}{u^2 q^2 + (\frac{1}{2}q^2 + \vec{k} \cdot \vec{q})^2}. \quad (\text{B6})$$

It is simple to show that the Pauli principle restriction can be dropped in this case and we get the useful representation

$$Q_q^{\pm}(u) = \int d^3k f_k^{\pm} \frac{2(\frac{1}{2}q^2 + \vec{k} \cdot \vec{q})}{u^2 q^2 + (\frac{1}{2}q^2 + \vec{k} \cdot \vec{q})^2}. \quad (\text{B7})$$

For small  $p$ , we can expand  $Q_q^{\pm}$  as follows:

$$Q_q^{\pm}(u) = Q_q(u) \pm p Q_q^{(1)}(u) + \frac{1}{2} p^2 Q_q^{(2)}(u) \pm \dots \quad (\text{B8})$$

Therefore, the dielectric function has the expansion

$$\epsilon_{\text{RPA}}(q, iqu) = 1 + (\lambda/\pi q^2) [Q_q(u) + \frac{1}{2} p^2 Q_q^{(2)}(u)] + O(p^4). \quad (\text{B9})$$

The term  $Q_q^{(2)}$  can be conveniently obtained from (B7) using (B4) since

$$\left. \frac{d^2}{dp^2} f_k^{\pm} \right|_{p=0} = \delta'(1 - k^3).$$

The integration is straightforward and gives

$$Q_q^{(2)}(u) = -\left(\frac{2}{5}\pi\right)(1/q)F(q, u), \quad (\text{B10})$$

where  $F(q, u)$  has already been defined in Eq. (2.38).

In the paramagnetic phase we have

$$\epsilon_{\text{RPA}}(q, iqu) = 1 + (\lambda/\pi q^2) Q_q(u). \quad (\text{B11})$$

The function  $Q_q(u)$  is well known<sup>41</sup> in literature

$$Q_q(u) = 2\pi \left\{ 1 - u \left[ \tan^{-1} \left( \frac{1 + \frac{1}{2}q}{u} \right) + \tan^{-1} \left( \frac{1 - \frac{1}{2}q}{u} \right) \right] + \frac{u^2 + 1 - \frac{1}{4}q^2}{2q} \ln \left( \frac{u^2 + (1 + \frac{1}{2}q)^2}{u^2 + (1 - \frac{1}{2}q)^2} \right) \right\}. \quad (\text{B12})$$

For small  $q$ , we have

$$Q_0(u) = 4\pi R(u), \quad (\text{B13})$$

with

$$R(u) = 1 - u \tan^{-1}(1/u).$$

#### ACKNOWLEDGMENTS

I am grateful to Professor Chanchal K. Majumdar for valuable comments and constant encouragement. I thank Professor Katuro Sawada for a valuable correspondence. I am grateful to Dr. I Rama Rao for a useful suggestion regarding the presentation of the material.

\*Based on the author's Ph.D. thesis, Bombay University (1976).

†Present address: Dept. of Physics, University of Hyderabad, "Golden Threshold," Nampalli Slaton Road, Hyderabad-500 001, India.

<sup>1</sup>C. Herring, *Magnetism*, edited by G. T. Rado and H. Suhl (Academic, New York, 1966), Vol. IV.

<sup>2</sup>B. Knecht, Ph.D. thesis (Cambridge University, 1974) (unpublished).

<sup>3</sup>T. Kushida, J. C. Murphy, and M. Hanabusa, *Phys. Rev. B* **13**, 5136 (1976); Fig. 6 of this paper seems to misrepresent the BS result which should be smaller than the RPA, rather than otherwise, as depicted.

<sup>4</sup>S. H. Vosko, J. P. Perdew, and A. H. Mac Donald, *Phys. Rev. Lett.* **35**, 1725 (1975).

<sup>5</sup>S. H. Vosko and J. P. Perdew, *Can. J. Phys.* **53**, 1385 (1975).

<sup>6</sup>C. Herring, in Ref. 1, p. 290.

<sup>7</sup>W. Kohn and L. J. Sham, *Phys. Rev.* **140**, A1133 (1965).

<sup>8</sup>An exhaustive list of electron gas calculations can be found in Ref. 3.

<sup>9</sup>R. S. Rao, C. K. Majumdar, B. S. Shastry and R. P. Singh, *Pramana* **4**, 45 (1975).

<sup>10</sup>R. Dupree and D. J. W. Geldart, *Solid State Commun.* **9**, 145 (1971).

<sup>11</sup>U. von Barth and L. Hedin, *J. Phys. C* **5**, 1629 (1972).

<sup>12</sup>D. R. Hamann and A. W. Overhauser, *Phys. Rev.* **143**, 183 (1966).

<sup>13</sup>P. Vasishta and K. S. Singwi, *Solid State Commun.* **13**, 901 (1973).

<sup>14</sup>S. H. Vosko and A. H. Mac Donald (unpublished).

<sup>15</sup>K. A. Brueckner and K. Sawada, *Phys. Rev.* **112**, 328 (1958).

<sup>16</sup>M. Gell-Mann and K. A. Brueckner, *Phys. Rev.* **106**,

- 364 (1957); K. Sawada, *ibid.* 106, 372 (1957); K. Sawada, K. Brueckner, N. Fukuda, and R. Brout, *ibid.* 108, 507 (1957).
- <sup>17</sup>J. Hubbard, Proc. R. Soc. A 243, 336 (1957).
- <sup>18</sup>C. Herring, in Ref. 1, p. 65.
- <sup>19</sup>C. Herring, in Ref. 1, p. 35, Eq. (3.1).
- <sup>20</sup>P. Nozières, *Theory of Interacting Fermi Systems* (Benjamin, New York, 1966), Chap. 1.
- <sup>21</sup>C. Herring, in Ref. 1, Sec. III.
- <sup>22</sup>T. M. Rice, Ann. Phys. (N.Y.) 31, 100 (1965).
- <sup>23</sup>G. Baym and L. P. Kadanoff, Phys. Rev. 124, 287 (1961).
- <sup>24</sup>P. Nozieres, in Ref. 20, Chap. 6.
- <sup>25</sup>J. Lam, Phys. Rev. B 5, 1254 (1972).
- <sup>26</sup>We would like to mention that Ref. 25 came to our attention (through Ref. 3) only after we started writing this paper. Incidentally, this also explains why the result L-RPA in Fig. 6 of Ref. 3 agrees with that of DG, VBH, and HO.
- <sup>27</sup>A. L. Fetter and J. D. Walecka, *Quantum Theory of Many Particle Systems* (McGraw-Hill, New York, 1971).
- <sup>28</sup>See, for example, A. L. Fetter and J. D. Walecka, in Ref. 27, p. 105.
- <sup>29</sup>This follows from the definition  $\mu = dE(h)/dN$  since the energy  $E$  can only be a function of  $h^2$ .
- <sup>30</sup>D. F. Du Bois, Ann. Phys. (N.Y.) 7, 174 (1959); 8, 24 (1959).
- <sup>31</sup>See, for example, A. L. Fetter and J. D. Walecka, in Ref. 25, p. 109.
- <sup>32</sup>In order to get good convergence, the integration was divided into three regions corresponding to  $0 \leq q \leq 1$ ;  $1 < q \leq 2$ ;  $2 < q$  and each rectangle scaled back into a square.
- <sup>33</sup>See, for example, A. L. Fetter and J. D. Walecka, in Ref. 25, p. 32, problem 1.5 (a).
- <sup>34</sup>K. Sawada (private communication); the identity follows on expressing
- $$\frac{d^2 f(x, x)}{dx^2} \Big|_{x=1} \text{ and } \frac{df(x, x)}{dx} \Big|_{x=1}$$
- in terms of partial derivatives of  $f(x, y)$  with respect to  $x$  and  $y$  and comparing the expressions.
- <sup>35</sup>*Handbook of Mathematical Functions*, edited by M. Abramowitz and I. Stegun (Dover, New York, 1965), pp. 892-893.
- <sup>36</sup>M. Gell-Mann, Phys. Rev. 106, 364 (1957).
- <sup>37</sup>D. J. W. Geldart and S. H. Vosko, Can. J. Phys. 44, 2137 (1966).
- <sup>38</sup>S. K. Joshi and A. K. Rajagopal, Adv. Solid State Phys. 22, 159 (1968), Appendix B; A. K. Rajagopal, Prāmana 4, 140 (1975).
- <sup>39</sup>B. S. Shastry, S. S. Jha, and A. K. Rajagopal, Phys. Rev. B 9, 2000 (1974).
- <sup>40</sup>From Ref. 22; this paper contains some typographical errors. We recomputed some of the quantities to assure ourselves of this, and thereby obtained somewhat more accurate values of  $m^*/m$  and  $\kappa_F/\kappa$  in the Hubbard scheme.
- <sup>41</sup>E. Daniell and S. H. Vosko, Phys. Rev. 120, 2041 (1960).
- <sup>42</sup>P. Vasishta and K. S. Singwi, Phys. Rev. B 6, 875 (1972); 6, (E) 4883 (1972).
- <sup>43</sup>B. Sriram Shastry, Phys. Rev. Lett. 38, 449 (1977).