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Correlations in a two-dimensional electron system

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The correlation energy per particle (expressed in rydbergs) of a two-dimensional electron gas is calculated by summing the ring diagrams. For high densities, this is found to be of the form $C + Dr_s \ln r_s + O(r_s)$, where r_s is a dimensionless parameter such that r_s^{-2} is proportional to the number of electrons per unit area. The value of D is -0.172 and that of C is -0.38 ± 0.04, the latter involves a numerical evaluation. By the same methods, we have also calculated the difference in total energy of the nonmagnetic and ferromagnetic states and we find for $r_s > 2.3$ the system may be ferromagnetic. We have also obtained some exact relationships between the pair correlation function at zero separation and the asymptotic behavior of the structure factor and the momentum distribution function. These are of interest in relation to scattering experiments.

I. INTRODUCTION

The conduction electrons in a metal are traditionally described as a dense gas of electrons with a neutralizing uniform positive charge in three dimensions. Between 1950 and 1960, sophisticated methods were developed to study the various aspects of this model system. It was soon realized that a clear comparison between the experimental results and those derived from this model cannot be made. However, much intuition was developed concerning this system in three dimensions.[1] Recently, two physical systems have come to be known as being essentially a two-dimensional version of the above electron-gas model with continuously variable density. They are electrons confined to the surface of liquid helium and to the interface of metal-oxide-semiconductor sandwiches. They seem to be more closely describable by the electron-gas model than the conduction electrons in metals in three dimensions, and for this reason there is much interest in calculating various properties of this two-dimensional system using the sophisticated methods developed twenty years ago. There are many surprises here. The dispersion of the plasmons in this system goes to zero for long wavelengths in contrast to the three-dimensional (3-D) situation. This has been experimentally confirmed.[2] Zia[3] calculated the correlation energy of a high-density electron gas in two dimensions based on the Gell-Mann and Brueckner method[4] developed earlier for the corresponding 3-D system. Zia has made several errors in his calculation as we shall show in the present paper. The correlation energy per particle in rydbergs approaches the form $C + Dr_s \ln r_s$, where r_s is the conventional dimensionless electron gas parameter and r_s^{-2} is proportional to the number density per unit area of the system. Zia concluded that D is negligible and thus C dominates. He found $C = -0.021 \pm 20\%$ and $D = +2.2 \times 10^{-4}$. We find that his D ought to be $8\pi^4$ times larger and has a negative sign. For very low densities, it is surmised as in three dimensions that this system may crystallize into a Wigner solid.[2,5] One of us[6] estimated that for intermediate densities, the system may perhaps exhibit ferromagnetism just as Bloch found in the 3-D system. One of us[7] has also computed the effects of exchange contributions to the plasmon dispersion etc. There are various other many-body aspects of these two systems that have been studied and one may refer to the conference report cited in Ref. 2 for information concerning them.

The plan of the present paper is to set up the correct Gell-Mann–Brueckner approach to the correlation energy problem in Sec. II for a magnetically polarized electron system. A relation between the paramagnetic and the fully-saturated-ferromagnetic state correlation energies is established similar to the one for the 3-D case given by Misawa.[8] In Sec. III, we carry out the calculation of the correlation energy of the high-density system for the paramagnetic state. In the same section, we also mention an alternate theory of the correlation energy based on the dielectric-function approach. This method is very physical in that it brings out certain aspects of the plasmon and particle-hole states explicitly. We derive an expression for the cutoff wave vector for the plasmon, beyond which it will decay into a particle-hole pair.

In Sec. IV, we give certain exact relationships concerning the pair correlation function, the structure factor, and the momentum distribution function for the two-dimensional (2-D) system, similar to the ones derived by the second author for the 3-D system.[9,10] In Sec. V we give a summary of the results derived in this paper.

II. CORRELATION ENERGY OF A POLARIZED ELECTRON GAS

We first establish the notation used in this work. We use units where $\hbar$, the Planck constant, divided by 2π is set equal to unity. The mean radius per particle of the system with the total number of electrons N confined to the surface area S is defined by the dimensionless parameter r_s,

$$\frac{S}{N} = \pi r_s^2 a_0^2, \quad a_0 = \frac{1}{me^2} \text{ is the Bohr radius.} \tag{1}$$

Here m is the mass and e is the charge of the electron. The Fermi momentum for the noninteracting system for spin σ is $k_{F\sigma}$ and is such that

$$[S/(2\pi)^2]\,\pi(k_{F\uparrow}^2 + k_{F\downarrow}^2) = N. \tag{2}$$

If ζ is the relative magnetization of the system, $0 \le \zeta \le 1$, we define

$$k_{F\uparrow} = k_F(1+\zeta)^{1/2}, \quad k_{F\downarrow} = k_F(1-\zeta)^{1/2}, \tag{3}$$

so that

$$k_F^2/2\pi = N/S. \tag{4}$$

Combining (1) and (4) we thus have the relation

$$\alpha r_s a_0 k_F = 1, \quad \text{where } \alpha = 1/\sqrt{2}. \tag{5}$$

The Hamiltonian of this system of electrons is

$$H = \sum_{k\sigma} \frac{k^2}{2m} C_{k\sigma}^\dagger C_{k\sigma} + \frac{1}{2} \sum_q \sum_{k\sigma} \sum_{k'\sigma'} V(q)\, C_{k+q\sigma}^\dagger C_{k'-q\sigma'}^\dagger C_{k'\sigma'} C_{k\sigma}, \tag{6}$$

where the wave vector $\vec{k}$ is two dimensional. $V(q)$ is the Fourier transform of the 2-D interaction potential between electrons (e^2/r_{12}) and is

$$V(q) = 2\pi e^2/|\vec{q}|. \tag{7}$$

$C_{k\sigma}, C_{k'\sigma}^\dagger$ obey the usual anticommutation rules. The ground state of the noninteracting system is the filled Fermi sea defined by

$$\Phi_0 = \prod_{\substack{k\sigma \\ (k<k_{F\sigma})}} C_{k\sigma}^\dagger |0\rangle. \tag{8}$$

The average kinetic energy per particle of the system is given by

$$\frac{T}{N} = \frac{S}{N} \sum_\sigma \int_{|\vec{k}|<k_{F\sigma}} \frac{k^2}{2m} \frac{d^2k}{(2\pi)^2} = \frac{k_F^2}{4m}(1+\zeta^2),$$

or expressed in rydbergs, using the relations (4) and (5),

$$k_F^2/2m = 1/\alpha^2 r_s^2, \tag{9}$$

we have

$$T/N = (1+\zeta^2)/2\alpha^2 r_s^2. \tag{10}$$

The first-order interaction energy per particle is the Hartree-Fock energy and is given in a convenient form:

$$\frac{E_1}{N} = -\frac{1}{2}\left(\frac{S}{(2\pi)^2}\right)^2 \frac{e^2}{S} \times \sum_\sigma \int_{|k_1|<k_{F\sigma}} d^2k_1 \times \int_{|k_2|<k_{F\sigma}} d^2k_2 \times \int \frac{d^2r}{|\vec{r}|} e^{i(\vec{k}_1-\vec{k}_2)\cdot\vec{r}}. \tag{11}$$

Doing the k_1, k_2 integrations first, using the identities

$$\int_{|k|<k_{F\sigma}} d^2k\, e^{i\vec{k}\cdot\vec{r}} = \int_0^{k_{F\sigma}} k\,dk\, 2\pi J_0(kr) = 2\pi k_{F\sigma} \frac{J_1(k_{F\sigma}r)}{r} \tag{12a}$$

and

$$\int_0^\infty \frac{d^2r}{|\vec{r}|} \frac{J_1^2(k_{F\sigma}r)}{|\vec{r}|^2} = 2\pi k_{F\sigma} \frac{4}{3\pi}, \tag{12b}$$

we obtain

$$E_1/N = -(4/3\pi\alpha r_s)[(1+\zeta)^{3/2} + (1-\zeta)^{3/2}]. \tag{13}$$

The second-order interaction energy per particle is given by

$$\frac{E_2}{N} = -\frac{1}{8\pi^3} \sum_{\sigma_1\sigma_2} \int d^2q \int d^2k_1 \int d^2k_2\; f_{\sigma_1}(k_1) f_{\sigma_2}(k_2)[1 - f_{\sigma_1}(\vec{k}_1+\vec{q})] \times [1 - f_{\sigma_2}(\vec{k}_2+\vec{q})]\left(\frac{1}{q^2} - \delta_{\sigma_1\sigma_2} \frac{1}{q|\vec{q}+\vec{k}_1+\vec{k}_2|}\right) \frac{1}{q^2 + \vec{q}\cdot(\vec{k}_1+\vec{k}_2)}. \tag{14}$$

Here $f_\sigma(k)$ stands for the usual Fermi function which at $T=0$ K, is just a step function. All the momenta here are scaled by k_F so that

$$f_\uparrow(k)=\Theta(k-(1+\zeta)^{1/2}),\quad f_\downarrow(k)=\Theta(k-(1-\zeta)^{1/2}), \tag{15}$$

where

$$\Theta(x)=\begin{cases}1 & \text{if } x<0,\\ 0 & \text{if } x>0.\end{cases}$$

The first term in (14) is the direct term and the second is an exchange contribution. E_2/N in rydbergs is independent of r_s. It may be further noted that the exchange term in E_2/N, because of the condition $\delta_{\sigma_1\sigma_2}$, *is found to be independent of magnetization*, ζ, as is seen by a simple scaling of the momentum vectors for each of the up and down spins and then adding them up. We call this $E_2^{(b)}/N$:

$$\frac{E_2^{(b)}}{N}=\frac{1}{4\pi^3}\int d^2q\int d^2k_1\int d^2k_2\, f(k_1)f(k_2)[1-f(\vec{k}_1+\vec{q})][1-f(\vec{k}_2+\vec{q})]\ \frac{1}{q\,|\vec{q}+\vec{k}_1+\vec{k}_2|}\ \frac{1}{q^2+\vec{q}\cdot(\vec{k}_1+\vec{k}_2)}\,. \tag{16}$$

Here $f(k)$ is the same as (15) with $\zeta=0$. Note that there is no divergence in $E_2^{(b)}/N$ or in the direct term in contrast to the 3-D calculation. Following Gell-Mann and Brueckner,[4] the direct term in the second-order energy is called the lowest-order ring diagram and will be denoted by $E_2^{(r)}/N$ and is expressed in the form

$$\frac{E_2^{(r)}}{N}=-\frac{1}{4\pi^2\alpha^2r_s^2}\frac{(-1)^2}{2}\int_{-\infty}^{\infty}du\int d^2q\,|\vec{q}|\left(\frac{\alpha r_s}{2\pi q}[Q_{q\uparrow}(u)+Q_{q\downarrow}(u)]\right)^2, \tag{17}$$

where

$$Q_{q\sigma}(u)=\int d^2k\int_{-\infty}^{\infty}dt\,e^{-|t|(q^2/2+\vec{q}\cdot\vec{k})}\,e^{ituq}f_\sigma(k)[1-f_\sigma(k+q)], \tag{18}$$

with $f_\sigma(k)$ defined as in Eq. (15). Note that $Q_{q\sigma}(u)$ is real and even in u. The contribution from the ring diagrams in the nth order is given by

$$\frac{E_n^{(r)}}{N}=-\frac{1}{4\pi^2\alpha^2r_s^2}\frac{(-1)^n}{n}\int_{-\infty}^{\infty}du\int d^2q\,|\vec{q}|\left(\frac{\alpha r_s}{2\pi q}[Q_{q\uparrow}(u)+Q_{q\downarrow}(u)]\right)^n. \tag{19}$$

For $n\geq 3$, observe that $E_n^{(r)}/N$ is divergent for small q. Summing over all the ring diagrams then, we obtain a closed form expression for the energy of the system:

$$\frac{E^{GB}}{N}=\frac{1+\zeta^2}{2\alpha^2r_s^2}-\frac{4}{3\pi\alpha r_s}[(1+\zeta)^{3/2}+(1-\zeta)^{3/2}]+\frac{1}{4\pi^3}\int d^2q\int d^2k_1\int d^2k_2\,\frac{f(k_1)f(k_2)[1-f(\vec{k}_1+\vec{q})][1-f(\vec{k}_2+\vec{q})]}{q\,|\vec{q}+\vec{k}_1+\vec{k}_2|[q^2+\vec{q}\cdot(\vec{k}_1+\vec{k}_2)]}$$
$$+\frac{1}{4\pi^2\alpha^2r_s^2}\int_{-\infty}^{\infty}du\int d^2q\,|\vec{q}|\left[\ln\left(1+\frac{\alpha r_s}{2\pi q}[Q_{q\uparrow}(u)+Q_{q\downarrow}(u)]\right)-\frac{\alpha r_s}{2\pi q}[Q_{q\uparrow}(u)+Q_{q\downarrow}(u)]\right]. \tag{20}$$

The last term in Eq. (20) is the ring contribution to the correlation energy of the system and is denoted here by $E_c^{(r)}(\zeta;r_s)/N$.

We will now establish a relationship between $E_c^{(r)}(\zeta=1;r_s)$ and the $\zeta=0$ (paramagnetic) energy, following the lines of Misawa who found a similar relation for the 3-D case. Note that for $\zeta=0$, we have

$$\frac{E_c^{(r)}(0;r_s)}{N}=\frac{1}{4\pi^2\alpha^2r_s^2}\int_{-\infty}^{\infty}du\int d^2q\,|\vec{q}|\left[\ln\left(1+\frac{\alpha r_s}{\pi q}Q_q(u)\right)-\frac{\alpha r_s}{\pi q}Q_q(u)\right], \tag{21}$$

and for $\zeta=1$,

$$\frac{E_c^{(r)}(1;r_s)}{N}=\frac{1}{4\pi^2\alpha^2r_s^2}\int_{-\infty}^{\infty}du\int d^2q\,|\vec{q}|\left[\ln\left(1+\frac{\alpha r_s}{2\pi q}Q_{q\uparrow}(u)\right)-\frac{\alpha r_s}{2\pi q}Q_{q\uparrow}(u)\right], \tag{22}$$

where

$$Q_{q\uparrow}(u)=\int d^2k\int_{-\infty}^{\infty}dt\exp\left[-|t|\left(\frac{q^2}{2}+\vec{q}\cdot\vec{k}\right)\right]e^{ituq}f_{\uparrow}(k)[1-f_{\uparrow}(\vec{k}+\vec{q})]\,.$$

In view of Eqs. (3) and (15), scale $\vec{k},\vec{q},t,u$ as follows:

$$\vec{k}\to 2^{1/2}\vec{k},\quad \vec{q}\to 2^{1/2}\vec{q},\qquad t\to\tfrac{1}{2}t,\quad u\to 2^{1/2}u,\tag{23}$$

and obtain

$$Q_{2^{1/2}q\uparrow}(2^{1/2}u)=Q_q(u)\,,\tag{24}$$

and so using (23) and (24) in Eq. (22) we get

$$\frac{E_c^{(r)}(1;r_s)}{N}=\frac{1}{4\pi^2\alpha^2r_s^2}\,4\int_{-\infty}^{\infty}du\int d^2q\,|\vec{q}|\left[\ln\left(1+\frac{\alpha r_s}{2\pi 2^{1/2}q}\,Q_q(u)\right)-\frac{\alpha r_s}{2\pi 2^{1/2}}\,Q_q(u)\right].$$

Hence,

$$\frac{E_c^{(r)}(1;r_s)}{N}=\tfrac{1}{2}\,E_c^{(r)}\left(0;\frac{r_s}{2^{3/2}}\right)\Big/N\,.\tag{25}$$

This result is similar to the one derived by Misawa for the 3-D system, where the scale factors are different.[8] We find the ferromagnetic state to be lower in energy compared to the paramagnetic state for $r_s>2.3$. This result is of course speculative because it is based on a high-density expansion. In the Hartree-Fock theory, this happened for $r_s>2$. This should be contrasted with what happened in the 3-D case, namely, $r_s>6.1$ (Misawa's original result that $r_s>7.4$ contains a numerical error) compared to the Hartree-Fock result, $r_s>5.45$.

An explicit evaluation of $Q_{q\sigma}(u)$ is possible. Here we give it for small q:

$$Q_{q\uparrow}(u)\equiv Q_q(u;\zeta)\quad\text{and}\quad Q_{q\downarrow}(u)\equiv Q_q(u;-\zeta)\,,\tag{26}$$

where it is enough if we know $Q_q(u;\zeta)$ for $u>0$ and so

$$Q_q(u;\zeta)=\frac{1}{q}\int_0^{k_{F\uparrow}}k\,dk\int_0^{2\pi}d\theta\,\frac{q+2k\cos\theta}{u^2+(\frac{1}{2}q+k\cos\theta)^2}\,.\tag{27}$$

In the high-density limit, we need the small q limit of Eq. (27) and it is given by

$$Q_q(u;\zeta)=\begin{cases}2\pi R(u') & \text{for } 0\le q\le(1+\zeta)^{1/2},\\ & u'=u/(1+\zeta)^{1/2},\\ 0 & \text{otherwise,}\end{cases}\tag{28}$$

where

$$R(u)=1-|u|/(u^2+1)^{1/2}\,.\tag{29}$$

III. CORRELATION ENERGY OF A PARAMAGNETIC ELECTRON SYSTEM–HIGH-DENSITY LIMIT

We will now discuss in detail the calculation of $E^{GB}(\zeta=0;r_s)/N$. We will first use (24) and (26) to make a few comments in relation to the work of Zia. We will then mention an alternative, equivalent expression for $E^{GB}(\zeta=0;r_s)/N$ in terms of the dielectric function calculated in the random-phase approximation.

In this case $\zeta=0$ and we have

$$\frac{E^{GB}(\zeta=0;r_s)}{N}=\frac{1}{2\alpha^2r_s^2}-\frac{8}{3\pi\alpha r_s}+E_2^{(b)}+\frac{1}{2\pi\alpha^2r_s^2}\int_{-\infty}^{\infty}du\int dq\,|\vec{q}|^2\left[\ln\left(1+\frac{\alpha r_s}{\pi q}\,Q_q(u)\right)-\frac{\alpha r_s}{\pi q}\,Q_q(u)\right].\tag{30}$$

In the high-density limit, we may use the $q\to 0$ limit of $Q_q(u)$ to evaluate the $r_s\ln r_s$ term in the correlation energy. Then Eq. (30) can be reduced further to the form

$$\frac{E^{GB}(\zeta=0;r_s)}{N}\simeq\frac{1}{2\alpha^2r_s^2}-\frac{8}{3\pi\alpha r_s}+E_2^{(b)}+\frac{1}{6\pi\alpha^2r_s^2}\int_{-\infty}^{\infty}du\left[\ln(1+2\alpha r_sR)-2\alpha r_sR-(2\alpha r_sR)^2+(2\alpha r_sR)^3\ln\left(1+\frac{1}{2\alpha r_sR}\right)\right].\tag{31}$$

Isolating the most divergent part, we finally obtain

$$\frac{E^{GB}(\zeta=0;r_s)}{N} \underset{(r_s\to 0)}{\simeq} \frac{1}{2\alpha^2 r_s^2} - \frac{8}{3\pi\alpha r_s} + (E_2^{(b)} + E_2^{(r)}) - \frac{2\sqrt{2}}{3\pi}(10-3\pi) r_s \ln r_s + O(r_s) . \tag{32}$$

In evaluating (31), we need an integral over $R^3(u)$ which is found to be

$$\int_{-\infty}^{\infty} du\, R^3(u) = 10 - 3\pi .$$

In (32), the constant terms, independent of r_s have been isolated and as noted earlier, these are the second-order terms, $E_2^{(r)} + E_2^{(b)}$ given by Eqs. (16) and (17) (with $n=2$). These integrals must be evaluated without approximation to obtain the constant term and this can only be done on a computer. The result of a Monte Carlo calculation is

$$\begin{aligned} (E_2^{(b)} + E_2^{(r)})/N &= -(0.38 \pm 0.04), \\ E_2^{(b)}/N &= 0.21 \pm 0.02 . \end{aligned} \tag{33}$$

Zia's result differs from ours in the following respects: (i) Zia's second term, the lowest-order exchange contribution is a factor of 2 smaller; (ii) our third term, the second-order exchange energy, independent of r_s is -0.38 ± 0.04, not -0.021; and (iii) Zia's $r_s \ln r_s$ term is $8\pi^4$ too small and has a minus sign. We thus have

$$\begin{aligned} E^{GB}(r_s)/N \sim 1/r_s^2 - 1.2/r_s - 0.38 \\ - 0.172 r_s \ln r_s + O(r_s) . \end{aligned} \tag{34}$$

The frequency and wave-vector-dependent longitudinal dielectric function for this system has been calculated by Stern in the random-phase approximation.[11] Using this we can express the correlation energy of this system due to contributions from all the ring diagrams as in the 3-D case.[1,4] Further, we may rewrite this in terms of a zero point plasmon contribution and a scattering contribution to the correlation energy. The plasmon dispersion relation is, in this approximation, given by [$\mathrm{Re}\,\epsilon_L(q;\omega)=0$ and $\mathrm{Im}\,\epsilon_L = 0$]

$$\begin{aligned} 1 = 2\frac{m^2e^2}{q^2}\Bigg\{ &\Theta\left(\frac{q^2k_f^2}{m^2} - \left(\omega_{pl} + \frac{q^2}{2m}\right)^2\right) \mathrm{sgn}\left(\omega_{pl} + \frac{q^2}{2m}\right) \\ &\times \left[\left(\omega_{pl} + \frac{q^2}{2m}\right)^2 - \frac{q^2k_F^2}{m^2}\right]^{1/2} \\ &- \Theta\left(\frac{q^2k_F^2}{m^2} - \left(\omega_{pl} - \frac{q^2}{2m}\right)^2\right) \mathrm{sgn}\left(\omega_{pl} - \frac{q^2}{2m}\right) \\ &\times \left[\left(\omega_{pl} - \frac{q^2}{2m}\right)^2 - \frac{q^2k_F^2}{m^2}\right]^{1/2} - \frac{q^2}{m}\Bigg\} . \end{aligned} \tag{35}$$

The cutoff wave vector q_{max} beyond which the plasmons are unstable towards electron-hole pairs is obtained when

$$\omega_{pl}(q_{max}) = q^2{}_{max}/2m + q_{max}k_F/m \tag{36}$$

in Eq. (35), and we obtain

$$q_{max}^2 = 2me^2\left[(q_{max}^2 + 2q_{max}k_F)^{1/2} - q_{max}\right] . \tag{37}$$

This again differs from Zia's expression; he gives $\frac{1}{2}me^2$ on the right-hand side of Eq. (37). In view of the complete equivalence of the final result for the correlation energy via the random-phase-approximation dielectric function and the Gell-Männ–Brueckner approach, we shall not give these expressions here.

IV. PAIR-CORRELATION FUNCTION AND THE STRUCTURE FACTOR

When two electrons are separated by a short distance, the physics which governs their behavior becomes a two-particle problem, and some exact relations can be obtained in the limit of zero interparticle separation.[9,10] The results obtained here are valid only for a strictly 2-D electron gas. In real systems with a nonzero width w, the results remain approximately valid for values of interparticle separations and inverse wave vectors which are larger than w but considerably less than $r_s a_0$.

The pair distribution function is proportional to the probability of finding two electrons separated by a distance r. This function is normalized to 1 for large r. For small r, properties of $g(r)$ can be obtained from the square of an effective two-electron wave function $\psi(\vec{r})$. This wave function must be a solution to a Schrödinger equation which, for two dimensions, has the form

$$\left[-\frac{1}{2\mu}\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r}\right) + \frac{e^2}{r}\right]\psi(r) = \epsilon\psi(r) , \tag{37}$$

where μ is the reduced mass of the two-electron pair equal to one-half the electron mass. No angular-momentum terms appear in Eq. (37) because only the s-state portion of $\psi(r)$ contributes significantly to $g(r)$ for small r. The term on the right-hand side of Eq. (37) includes complicated many-body effects, but since these effects are finite as $r \to 0$, the coefficient of the singular terms on the left-hand side of the equation may be set equal to zero. Expanding $\psi(r)$ as a power series in r yields

$$\psi(r) \approx 1 + (1/a_0)r + \cdots . \tag{38}$$

Since $g(r)$ is proportional to $\psi^*\psi$,

$$\left.\frac{dg(r)}{dr}\right|_{r\to 0} = \frac{2}{a_0} g(0) , \tag{39}$$

where a_0 is the Bohr radius. This result differs

from a corresponding relation in three dimensions[9,10] only by a factor of 2 which comes from the different form for the Laplacian.

The structure factor $S(q)$ is essentially the Fourier transform of the pair-correlation function $g(r)$. Following the notation of Pines,[1]

$$1-g(r)=\frac{1}{N-1}\sum_{q} e^{i\vec{q}\cdot\vec{r}}[1-S(q)], \tag{40}$$

or, in two dimensions,

$$1-g(r)=\begin{cases}\dfrac{1}{2\pi k_F^2}\displaystyle\int e^{i\vec{q}\cdot\vec{r}}[1-S(q)]\,d^2q\,,\\[2ex] \dfrac{1}{k_F^2}\displaystyle\int_0^\infty J_0(qr)[1-S(q)]\,q\,dq\,.\end{cases} \tag{41}$$

The large-q behavior of $S(q)$ leads to the discontinuous derivative of $g(r)$ as r approaches zero. The appropriate behavior of $g(r)$ is produced by an asymptotic $1/q^3$ dependence of $[1-S(q)]$.

We define the function $\delta(q)$ by

$$\delta(q)=1-S(q)-\gamma/q(1+q^2)\,, \tag{42}$$

where

$$\gamma=\lim_{q\to\infty}\{q^3[1-S(q)]\}. \tag{43}$$

With this choice of γ, $\delta(q)$ vanishes so rapidly for large q that it does not contribute to the derivative at $g(r)$ at the origin. Using Eqs. (41) and (42),

$$\left.\frac{dg(r)}{dr}\right|_{r\to 0}=-\lim_{r\to 0}\left(\frac{d}{dr}\frac{\gamma}{k_F^2}\int_0^\infty\frac{J_0(qr)}{q^2+1}\,dq\right)$$

$$=\frac{-\pi\gamma}{2k_F^2}\lim\left(\frac{d}{dr}[I_0(r)-L_0(r)]\right). \tag{44}$$

Here $I_0(r)$ is a Bessel function of imaginary argument and $L_0(r)$ is a Struve function.

Only the Struve function varies linearly with r for small r,

$$L_0(r)=2r/\pi+\cdots. \tag{45}$$

Hence,

$$\left.\frac{dg(r)}{dr}\right|_{r\to 0}=\frac{\gamma}{k_F^2} \tag{46}$$

and

$$g(0)=\frac{a_0}{2k_F^2}\lim_{q\to\infty}\{q^3[1-S(q)]\}. \tag{47}$$

The probability of finding an electron of wave vector $\vec{k}$, $n(\vec{k})$, is given by (ψ being the normalized many-electron wave function)

$$n(k)=\frac{N}{S}\int e^{i\vec{k}\cdot(\vec{r}-\vec{r}')}\psi^*(\vec{r},\vec{r}_2,\ldots,r_N)\times\psi(r',r_2,\ldots,r_N)d^2r\,d^2r'\prod_{i=2}^{N}d^2r_i; \tag{48}$$

the probability of finding two electrons at points $\vec{r}_1$ and $\vec{r}_2$ is

$$g(\vec{r}_1,\vec{r}_2)=N(N-1)\int\psi^*(\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_N)\times\psi(\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_N)\prod_{i=3}^{N}d^2r_i; \tag{49}$$

and the pair-correlation function is

$$g(r)=\frac{S}{N^2}\int g(\vec{r}_1+\vec{r},\vec{r}_1)\,d^2r_1\,. \tag{50}$$

In (50), the normalization S/N^2 is chosen to make $g(r)\to 1$ for $r\to\infty$. The dominant contribution to $n(\vec{k})$ is produced by the kinks in ψ which occur at zero interparticle separation. In Eq. (48), the lowest-order terms in $1/k$ which contribute to $n(k)$ occur when both r and r' are near the same electronic coordinate. For large k,

$$n(k)=\frac{N(N-1)}{S}\int_{\Omega(\vec{r}_2)}e^{i\vec{k}\cdot(\vec{r}-\vec{r}')}\psi^*(\vec{r},\vec{r}_2,\ldots,\vec{r}_n)\times\psi(\vec{r}',\vec{r}_2,\ldots,\vec{r}_N)d^2r\,d^2r'\times\prod_{i=2}^{N}d^2r_i, \tag{51}$$

where $\int_{\Omega(\vec{r}_2)}$ means $\vec{r}$ and $\vec{r}'$ are near $\vec{r}_2$ and the additional factor of $N-1$ appears because the single coordinate ($\vec{r}_2$) was selected from $(N-1)$ indistinguishable possibilities. When $\vec{r}$ is near $\vec{r}_2$, ψ may be approximated by

$$\psi(r,r_2,\ldots,r_N)\approx\left(1+\frac{|\vec{r}-\vec{r}_2|}{a_0}\right)\psi(r\simeq r_2,r_2,\ldots,r_N)\,, \tag{52}$$

and $n(k)$ becomes

$$n(k)\simeq\left(\frac{N}{S}\right)^2 g(0)\left(\int e^{i\vec{k}\cdot\vec{r}}e^{-r/a_0}d^2r\right)^2 \tag{53}$$

or

$$n(k)\Rightarrow(N/S)^2[g(0)/a_0^2](2\pi)^2/k^6 \tag{54}$$

and

$$g(0)=\frac{a_0^2}{k_F^4}\lim_{k\to\infty}[k^6n(k)]. \tag{55}$$

From the x-ray and electron-scattering experi-

ments for large momentum transfers, one may obtain $S(q)$ and $n(k)$ and the results obtained here relate the large momentum limits of these to $g(0)$, the zero-range correlation function. Such measurements will yield valuable information concerning the zero-range correlation function, for example, deviations from the Hartree-Fock value of $g(0)$.

V. SUMMARY AND CONCLUDING REMARKS

Our main results are as follows: (i) Eq. (20), an expression for correlation energy of a polarized electron gas which includes the ring diagrams of all orders and first- and second-order exchange processes; (ii) the relation of Eq. (25) between the correlation energies of the paramagnetic and ferromagnetic states; (iii) the expression for the energy for high densities, Eq. (34). This corrects the result of Zia; (iv) we have shown that $r_s > 2.3$, ferromagnetic state is favored. This result is based on Eq. (25), the approximation given by Eqs. (28) and (29) and explicit numerical evaluation of Eq. (31). Compare this with the Hartree-Fock result,[6] $r_s > 2$; (v) Eq. (39) relating the discontinuity of the pair-correlation function to the value of this function for zero separation. This is exact; and (vi)

$$g(0) = \frac{a_0}{2k_F^2} \lim_{q\to\infty}\{q^3[1 - S(q)]\} = \frac{a_0^2}{k_F^4} \lim_{k\to\infty}[k^6 n(k)]\,. \tag{56}$$

This result may serve as an experimental measure of $g(0)$, the zero-range correlation function.

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[1]See, for instance, the collected papers on *The Many Body Problem*, edited by D. Pines (Benjamin, New York, 1961); and D. Pines, *Elementary Excitations in Solids* (Benjamin, New York, 1962), where an account of the comparison between theory and experiment are given.

[2]For a recent report on the various aspects of these two-dimensional systems, one may refer to the summary talk by F. Stern, Surf. Sci (to be published). This issue of Surf. Sci. has many papers on subject, being the Proceedings of an International Conference on the Electronic Properties of Quasi-Two-Dimensional Sytems held at Brown University in August 1975.

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