PHYSICAL REVIEW A VOLUME 9, NUMBER 6 JUNE 1974

Liquid-impurity correlations for Fermi systems*

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(Received 16 August 1973)

An attractive δ-function potential is introduced in a Fermi gas. The contribution to the liquid-impurity correlation function of bound states is calculated exactly in a Green's-function formalism. The exact results are compared with those obtained in a self-consistent approximation and the range of validity of the latter is discussed.

I. INTRODUCTION

The many-particle problem has been the major difficulty in the understanding of the physics of condensed matter. It has been the subject of an extensive literature for many years.[1]

Several theoretical techniques have improved the understanding of many-particle systems substantially, such as Green's functions, graphs, self-consistent-field theory, and so on. One of the most successful approaches in dealing with quantum liquids is the self-consistent-field approach of Singwi *et al.*,[2] which we shall abbreviate as SCA. We must remind the reader that Singwi's theory is one of the many self-consistent-field approximations in the literature, but owing to the extremely good results of the theory for the electron gas it is the one approximation which shall concern us in this paper.

The *ansatz* which allows the SCA has been discussed under several different forms but to give a brief account of the method we shall use the original, and to our understanding, the most intuitive one. The heart of the matter is to assume that long-range macroscopic fields can be dealt with semiclassically, as well as the correlation functions which generate them.

In order to obtain a self-consistent field acting on the one-particle distribution function one decouples, and this is the *ansatz,* the two-particle distribution function into a product of the two one-particle distribution functions times the static-pair-correlation function

$$f_2(\vec{r}_1,\vec{p}_1;\vec{r}_2,\vec{p}_2\,|\,t)=f_1(\vec{r}_1,\vec{p}_1;t)f_1(\vec{r}_2,\vec{p}_2;t)g(\vec{r}_1-\vec{r}_2)\,. \tag{1.1}$$

This decoupling scheme leads to an integral equation for $g(\vec{r})$ which can be solved by numerical methods.

The SCA was later extended by Sjölander and Stott[3] to deal with the case of the interaction of an electron gas with impurities. The method is very attractive and straightforward but, as the authors mention in their paper, has not been successful for positive impurities of infinite mass. Also, the calculated positron annihilation rate in metals broke down in a similar fashion to the more conventional T-matrix approaches; i.e., it shows an anomalous enhancement in the low-density region.[4]

A short time after the Sjölander and Stott paper, Bhattacharyya and Singwi[5] calculated again the positron annihilation rate in metals obtaining, through a slightly different *ansatz,* a very nice fit with the experimental data. It was not clear, nevertheless, if bound states could be accounted for in the theory and, more generally, when the SCA would be correct even in the absence of bound states.

In order to help clarify some of these problems a study has been carried out of a simple model system. The induced particle density has been calculated around a fixed δ-function potential in a noninteracting Fermi gas. For this system a closed-form expression can be obtained for the induced particle density and compared with the result of the SCA. In this way the validity of the approximate method may be tested.

A well-known problem of the three-dimensional δ-function attractive potential is that it must be renormalized in order to give finite results. This renormalization procedure and the solution for free particles is shown in Sec. II.

In Sec. III, a brief account of the SCA is presented, the renormalization is again discussed, and a closed solution is found.

In Sec. IV the exact Green's-function solution is found. Four cases are discussed for the renormalized δ potential. It is shown that the bound-state solution is outside the scope of the SCA. Moreover, only for weak repulsive potentials is the approximation correct but, in this case, it is exact up to second order in the interaction. In an intermediate region the SCA is not exact but may be a good approximation if the bound-state contribution is not preponderant. The case of an interacting Fermi system is briefly discussed in Sec. V, where the results are analyzed.

Numerical results for the SCA and for the exact Green's-function solution are compared and shown in several graphs.

II. δ POTENTIAL FOR FREE PARTICLES

The existence of bound states for the three-dimensional attractive δ potential is well established in the literature. Güttinger *et al.*[6] have shown that the bound-state problem is essentially connected to resonance effects and that for a three-dimensional attractive δ function, the existence of a bound state requires an interaction strength that goes to zero in such a way that resonance states are preserved in the limiting processes. In this section we rederive their results both for completeness of our exposition and for introducing the renormalization procedure, which must be performed in every step of our work.

Consider one particle, without spin, in the presence of an attractive, very sharply localized, potential $\phi(\vec{r})$ of strength A, which is put at the point $\vec{r}=0$, and is given by a δ function,

$$\phi(\vec{r}) = A\delta(\vec{r}) . \tag{2.1}$$

The Schrödinger equation for that particle in a real space is

$$-\nabla^2\psi(\vec{r}) + A\delta(\vec{r})\psi(\vec{r}) = E\psi(\vec{r}) . \tag{2.2}$$

Equation (2.2) may be rewritten in momentum space and solved for $\psi(\vec{p})$. (In this work we are using units which $2m = \hbar = 1$.) We obtain

$$\psi(\vec{p}) = \frac{A\sum_{p'}\psi(\vec{p}\,')}{E - p^2} . \tag{2.3}$$

If we add Eq. (2.3) for all $\vec{p}$'s, an implicit equation for E follows:

$$\frac{1}{A} = \sum_{p} \frac{1}{E - p^2} . \tag{2.4}$$

The right-hand side of this equation is divergent for all E's. However, this divergence may be eliminated by adding and subtracting into Eq. (2.4) a term

$$\sum_{p}^{K} \frac{1}{p^2} .$$

Then, we may rewrite Eq. (2.4) in terms of a renormalized interaction β as

$$\frac{1}{A} + \sum_{p=0}^{K} \frac{1}{p^2} = \sum_{p=0}^{K} \frac{E}{p^2(E-p^2)} + \sum_{p=K}^{\infty} \frac{1}{E-p^2} = \frac{1}{\beta} , \tag{2.5}$$

where $K \to \infty$ at the end of the calculations. From this last equation we find for the energy E of the bound state the expression

$$\frac{1}{A} + \frac{1}{2\pi^2} K = \frac{|E|^{1/2}}{2\pi^2} \tan^{-1}\left(\frac{K}{|E|^{1/2}}\right) + \sum_{p=K}^{\infty} \frac{1}{E-p^2} . \tag{2.6}$$

We now perform the limiting processes $A \to 0$ and $K \to \infty$ in such a way that

$$\lim_{A\to 0, K\to\infty}\left(\frac{1}{A} + \frac{1}{2\pi^2} K\right) = \frac{1}{\beta} , \tag{2.7}$$

where $1/\beta$ is finite and positive. Then, the energy for the bound state is given by

$$E_b = -16\pi^2/\beta^2 \tag{2.8}$$

for $\beta > 0$. If $\beta < 0$ there is no bound-state solution. In Fig. 1 we show schematically the graphical solution of Eq. (2.5) for $\beta > 0$.

If we define in a square well the potential as

$$V = 2AK^3 , \tag{2.9}$$

the condition that

$$\frac{1}{A} + \frac{1}{2\pi^2} K$$

be finite implies that $K/\lambda \to 1$, where λ is the wavelength of the bound state, $\lambda = 2\pi(E-V)^{-1/2}$, and $1/K$ is the range of the potential. Resonance states are thus preserved in the limiting processes, Eq. (2.7), with $1/\beta$ being a measure for the proximity to resonance.

III. SELF-CONSISTENT-FIELD APPROXIMATION

Recently, Singwi *et al.*[2] developed a new treatment for the dielectric function of metals for the metallic density range ($1 \leq r_s \leq 6$). (r_s is defined in the usual way, namely, $r_s = r_0/a_0$, where r_0 is the average particle distance and a_0 is the Bohr radius.) In their theory the short-range correlations, responsible for the local-field correction, are calculated in a self-consistent way, and the dielectric function becomes a functional of the electron-gas self-correlation function $g(\vec{r})$.

The *ansatz*, in the semiclassical case, replaces the two-particle distribution function in the Liouville equation for the one-particle distribution function $f(\vec{r}, \vec{p}\,|\,t)$ by

$$f_2(\vec{r}, \vec{p}; \vec{r}\,', \vec{p}\,'\,|\,t) = f_1(\vec{r}, \vec{p}\,|\,t) f_1(\vec{r}\,', \vec{p}\,'\,|\,t) g(\vec{r} - \vec{r}\,') , \tag{3.1}$$

thus making it possible to obtain a closed-form scheme for calculating the pair-correlation function $g(\vec{r})$ as follows.

The Fourier transform of $g(\vec{r})-1$ is

$$(1/\rho)[S(\vec{q})-1], \tag{3.2}$$

where ρ is the average density of the fluid and $S(\vec{q})$ is the static structure factor. The structure factor is related to the susceptibility of the fluid through the well-known relation

$$S(\vec{q})=-\frac{1}{\pi\rho}\int_0^\infty \mathrm{Im}[\chi(\vec{q},\omega)]\,d\omega\,. \tag{3.3}$$

With the *ansatz* used above, the susceptibility of the fluid becomes

$$\chi(\vec{q},\omega)=\frac{\chi_0(\vec{q},\omega)}{1-\psi(\vec{q})\chi_0(\vec{q},\omega)}, \tag{3.4}$$

where $\chi_0(\vec{q},\omega)$ is the susceptibility of a noninteracting system with the same mass, density, and statistics as the one under consideration. $\psi(\vec{q})$ is the self-consistent potential, given by

$$\psi(\vec{q})=\phi(\vec{q})+\frac{1}{\rho}\int\frac{d\vec{q}\,'}{(2\pi)^3}\,\frac{\vec{q}\cdot\vec{q}\,'}{q^2}\,\phi(\vec{q}\,')[S(\vec{q}-\vec{q}\,')-1] \tag{3.5}$$

and here $\phi(\vec{q})$ is the bare particle-particle interaction potential. The susceptibility is now a functional of $S(\vec{q})$ and the scheme is thus closed.

The SCA represents a definite improvement on the theory of the electron gas, several experimental results being explained theoretically from first principles, as the reader can verify in a large number of papers which use this theory as a starting point.[7]

Sjölander and Stott[3] have extended the theory for the case of two interacting systems of different particles, a and b, and again a self-consistent procedure was presented to calculate the cross-correlation function $g^{ab}(\vec{r})$. This new approach can be used to treat particles with infinite as well as finite masses with positive or negative charges.

If one of the systems, b say, is very dilute and has a very large mass, the calculation is simplified a great deal and the change of density $\langle\rho^a(\vec{q})\rangle$ of the system a around the b particle may be calculated, in a momentum space, simply as

$$\langle\rho^a(\vec{q})\rangle=\frac{\psi^{ab}(\vec{q})\chi_0^a(\vec{q},0)}{1-\psi^{aa}(\vec{q})\chi_0^a(\vec{q},0)}, \tag{3.6}$$

where $\chi_0^a(\vec{q},0)$ is the free a-particle susceptibility and $\psi^{ab}(\vec{q})$ is the self-consistent interaction given by

$$\psi^{ab}(\vec{q})=\phi^{ab}(\vec{q})\left(1+\int\frac{d\vec{q}\,'}{(2\pi)^3}\,\frac{\vec{q}\cdot\vec{q}\,'}{q^2}\,\gamma^{ab}(\vec{q}-\vec{q}\,')\right). \tag{3.7}$$

Here, $\gamma^{ab}(\vec{q})$ is related to the cross-correlation function $g^{ab}(\vec{r})$ by

$$\gamma^{ab}(\vec{q})=\int d\vec{r}\,e^{i\vec{q}\cdot\vec{r}}[g^{ab}(\vec{r})-1], \tag{3.8}$$

$\phi^{ab}(\vec{q})$ is the Fourier transform of the a-b interaction potential, and the induced density of the system a in terms of $\gamma^{ab}(\vec{q})$ is

$$\langle\rho^a(\vec{q})\rangle=\rho_0^a\gamma^{ab}(\vec{q})\,. \tag{3.9}$$

Looking at Eq. (3.9) we see that the induced density is now directly related to the cross-correlation function $g^{ab}(\vec{r})$ through the equilibrium density ρ_0^a.

To discuss the problem we have in mind, we assume an attractive δ interaction between a and b and neglect the interactions among a particles. Assuming an attractive δ interacting potential of

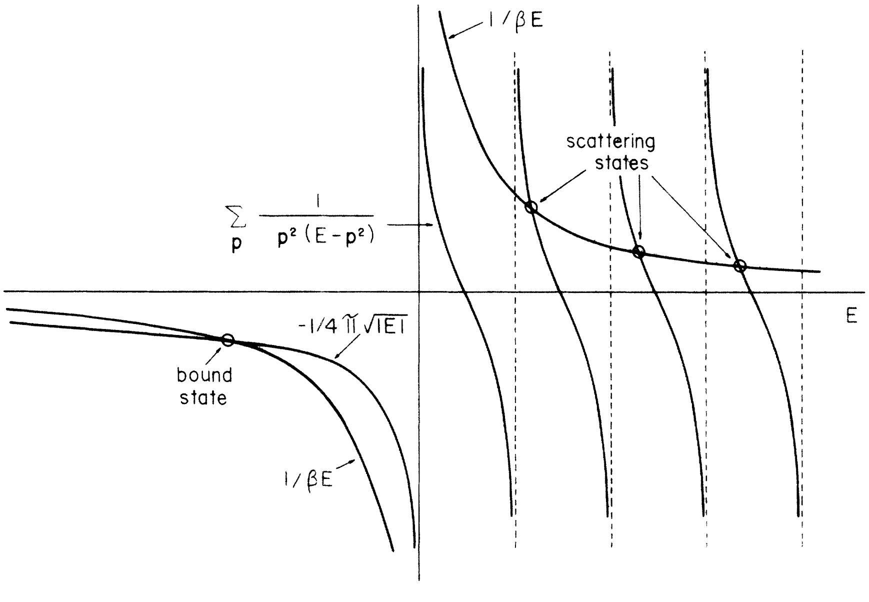

FIG. 1. Schematic graphical solutions of Eq. (2.5) for $\beta>0$. The two sides of that equation are plotted vs E. Its intersections give the scattering-state energies for $E>0$ and the bound-state energy for $E<0$.

strength A acting between a and b, we obtain the following equation for the induced density:

$$\langle\rho^a(\vec{q})\rangle = A\chi_0^a(\vec{q},0)\left(1+\frac{1}{2\pi^2\rho_0^a}\int dp\,p^2\langle\rho^a(\vec{p})\rangle\right). \tag{3.10}$$

This equation may be solved algebraically by integrating both sides in $\vec{q}$ and grouping the terms. We then have the result

$$\langle\rho^a(\vec{q})\rangle = \chi_0^a(\vec{q},0)\Big/\left(\frac{1}{A}-\frac{1}{2\pi^2\rho_0^a}\int dp\,p^2\chi_0^a(\vec{p},0)\right). \tag{3.11}$$

In Eq. (3.11) we see that the second term in the denominator is divergent, as $\chi_0^a(\vec{p},0)$ goes as p^{-2} for large p's. We may eliminate this divergence following the same procedure as in Sec. II, renormalizing the potential, defining β as

$$\frac{1}{\beta}=\frac{1}{A}-\frac{1}{2\pi^2\rho_0^a}\int_0^K dp\,p^2\chi_0^a(\vec{p},0), \tag{3.12}$$

so that at the end of the calculations we shall make $A\rightarrow 0$ and $K\rightarrow\infty$ in such a way that $1/\beta$ becomes finite. We end up with an induced density for a particles given by

$$\langle\rho^a(\vec{q})\rangle = \beta\chi_0^a(\vec{q},0). \tag{3.13}$$

We may now calculate $\langle\rho^a(\vec{r})\rangle$ by taking the inverse Fourier transform of Eq. (3.13),

$$\langle\rho^a(\vec{r})\rangle = \frac{\beta q_F^3}{2\pi^2 r}\int dq\,q\sin(qr)\chi_0^a(\vec{q},0). \tag{3.14}$$

Here q is taken in units of Fermi momentum q_F and r in terms of q_F^{-1}.

To clarify the r dependence of the induced density we separate the right-hand side of Eq. (3.14) into two parts which have different r behavior:

$$\langle\rho^a(\vec{r})\rangle = \frac{-\beta q_F^3\tau}{2\pi^2 r}\int dq\,\frac{\sin(qr)}{q}+\frac{\beta q_F^3}{2\pi^2 r}\int dq\,q\sin(qr)\times\left(\chi_0^a(\vec{q},0)+\frac{\tau}{q^2}\right), \tag{3.15}$$

where $\tau=2q_F/3\pi^2$. The first term in the right-hand side of Eq. (3.15) diverges as $1/r$ when $r\rightarrow 0$, while the second term is well behaved for all r's.

Finally we obtain an expression for the cross-correlation function,

$$g^{ab}(\vec{r}) = 1+\langle\rho^a(\vec{r})\rangle/\rho_0^a. \tag{3.16}$$

Inserting the induced density obtained in Eq. (3.15) into Eq. (3.16) we may write

$$g^{ab}(\vec{r}) = 1-\frac{\beta q_F^3\tau}{4\pi\rho_0^a r}+\frac{\beta q_F^3}{2\pi^2\rho_0^a r}\int dq\,q\sin(qr)\left(\chi_0^a(\vec{q},0)+\frac{\tau}{q^2}\right). \tag{3.17}$$

We calculated numerically $g^{ab}(\vec{r})$ assuming a noninteracting Fermi gas for several densities. In Fig. 2 we plot the numerical result of $[g^{ab}(\vec{r})-1]/\beta q_F$ vs $q_F r$ for $r_s=4$. For large values of r, $g^{ab}(\vec{r})$ exhibits an oscillatory behavior which is inserted in Fig. 2 expanded ×2 horizontally and ×40 vertically. Curves for other densities as well as for a-a interacting systems via a Coulomb potential were omitted since they do not differ substantially from the result shown in Fig. 2.

IV. GREEN'S-FUNCTION SOLUTION FOR THE δ-FUNCTION POTENTIAL

We briefly summarize the theory to be used in this section.[8] The standard problem of one-particle quantum theory is that of the free particle acted upon by a local potential $\phi(\vec{r})$. The Green's-function approach is known to be one of the most successful theoretical tools to deal with such problems. In general, one may solve, formally, the Green's-function equation for an arbitrary

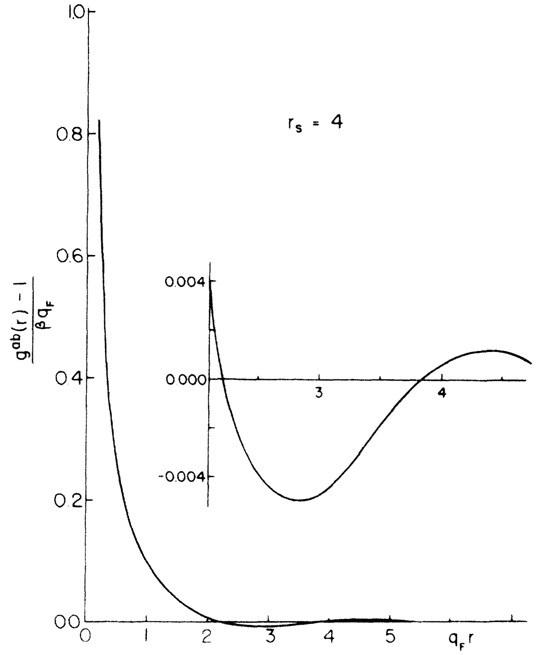

FIG. 2. $[g^{ab}(r)-1]/\beta q_F$ vs $q_F r$ for $r_s=4$. The insert shows the oscillatory part expanded ×2 horizontally and ×40 vertically.

system by the use of Dyson's equation,

$$G=G_0+G_0\Sigma G\,, \tag{4.1}$$

where G_0 is the free-particle propagator and Σ is the summation of all irreducible self-energy graphs, i.e., those which cannot be divided in two by the cut of just one particle line. In the simple case of an external potential acting on an assembly of noninteracting particles, Dyson's equation reduces to that of the one-particle problem with the free propagator G_0 being considered in the unperturbed noninteracting medium. Dyson's equation assumes the simple form

$$G=G_0+G_0\phi G\,, \tag{4.2}$$

which corresponds to the well-known Brillouin-Wigner perturbation series through the method of the resolvent.

We again assume an attractive δ potential acting on a noninteracting Fermion gas. We take this potential to be located at point $\vec{r}=0$. We now solve the problem using Dyson's equation for the exact Green's function of the gas in terms of the free-particle Green's function $G_0(\vec{r},\vec{r}\,',E)$ of the unperturbed noninteracting medium,

$$G(\vec{r},\vec{r}\,',E)=G_0(\vec{r},\vec{r}\,',E)+\int G_0(\vec{r},\vec{r}\,'',E)\phi(\vec{r}\,'')G(\vec{r}\,'',\vec{r}\,',E)\,d\vec{r}\,''\,, \tag{4.3}$$

where

$$\phi(\vec{r})=A\delta(\vec{r})\quad\text{with } A<0 \tag{4.4}$$

and

$$G_0(\vec{r},\vec{r}\,',E)=\int\frac{d\vec{p}}{(2\pi)^3}\,\frac{e^{i\vec{p}\cdot(\vec{r}-\vec{r}\,')}}{E-E_{\vec{p}}+i\eta_{\vec{p}}}\,, \tag{4.5}$$

with

$$\eta_{\vec{p}}=\eta>0\quad\text{if } |\vec{p}|>p_F$$
$$=-\eta\quad\text{if } |\vec{p}|<p_F\,.$$

Solving Eq. (4.3) for $G(\vec{r},\vec{r}\,',E)$, we find

$$G(\vec{r},\vec{r}\,',E)=G_0(\vec{r},\vec{r}\,',E)+\frac{AG_0(\vec{r},0,E)G_0(0,\vec{r}\,',E)}{1-AG_0(0,0,E)}\,. \tag{4.6}$$

We are interested in the density change of the gas due to the external potential. We are thus interested in finding $\delta G(\vec{r},\vec{r},E)$, which can be obtained directly from Eq. (4.6) as

$$\delta G(\vec{r},\vec{r},E)=G(\vec{r},\vec{r},E)-G_0(\vec{r},\vec{r},E)$$
$$=\frac{AG_0(\vec{r},0,E)G_0(0,\vec{r},E)}{1-AG_0(0,0,E)}\,. \tag{4.7}$$

We now define the Fourier transform of $\delta G(\vec{r},\vec{r},E)$:

$$\delta\tilde{G}(\vec{q},E)=\int d\vec{r}\,e^{-i\vec{q}\cdot\vec{r}}G(\vec{r},\vec{r},E) \tag{4.8}$$

or

$$\delta\tilde{G}(\vec{q},E)=\int\frac{d\vec{p}}{(2\pi)^3}\,\frac{\tilde{G}_0(\vec{p},E)\tilde{G}_0(\vec{p}+\vec{q},E)}{1/A-G_0(0,0,E)}\,, \tag{4.9}$$

where $\tilde{G}_0(\vec{p},E)$ is the Fourier transform of $G_0(\vec{r}-\vec{r}\,',E)$. The denominator of the right-hand side of Eq. (4.9) may be evaluated by noticing that for real E

$$G_0(0,0,E)=\int\frac{d\vec{p}}{(2\pi)^3}\,\frac{1}{E_{\vec{p}}}+P\int dE_{\vec{p}}\,\frac{EN(E_{\vec{p}})}{E_{\vec{p}}(E-E_{\vec{p}})}-i\delta_E\pi N(E)\,, \tag{4.10}$$

where P is the principal part of the integral, $N(E)$ is the density of states and δ_E is defined as

$$\delta_E=1\quad\text{for } E>E_F$$
$$=-1\quad\text{otherwise}\,.$$

For complex E we keep the complex integral representation as in Eq. (4.5) for $\vec{r}=\vec{r}\,'$.

$G_0(0,0,E)$ is divergent in the same way as the divergences found in Secs. II and III. We follow again the renormalization procedure, defining $1/\beta$ as

$$\lim_{A\to0,K\to\infty}\left(\frac{1}{A}+\int_0^K\frac{d\vec{p}}{(2\pi)^3}\,\frac{1}{E_{\vec{p}}}\right)=\frac{1}{\beta}\,. \tag{4.11}$$

Thus, Eq. (4.9) may now be rewritten as

$$\delta\tilde{G}(\vec{q},E)=\int\frac{d\vec{p}}{(2\pi)^3}\,\frac{1}{E-E_{\vec{p}}+i\eta_{\vec{p}}}\,\frac{1}{E-E_{\vec{p}+\vec{q}}+i\eta_{\vec{p}+\vec{q}}}\times\left(\frac{1}{\beta}-P\int dE_{\vec{p}}\,\frac{EN(E_{\vec{p}})}{E_{\vec{p}}(E-E_{\vec{p}})}-i\delta_E\pi N(E)\right)^{-1}\,. \tag{4.12}$$

The induced density is given by

$$\langle\rho(\vec{q})\rangle=-i\int\frac{dE}{2\pi}\,\delta\tilde{G}(\vec{q},E)\,. \tag{4.13}$$

We must therefore integrate Eq. (4.13) for all E's to obtain $\langle\rho(\vec{q})\rangle$. The integration is performed by closing the contour on the upper half of the complex plane, avoiding the cut $0<E<E_F$, as shown in Fig. 3, and encircling the pole E_b if $\beta>0$. Otherwise, no pole exists and the integration reduces to that around the cut.

If $\beta>0$, the contribution C_2 to $\langle\rho(\vec{q})\rangle$, I_1, is given by

$$I_1=-f(\vec{q},E_b)\bigg/\int_0^\infty dE_{\vec{p}}\,\frac{N(E_{\vec{p}})}{(E_b-E_{\vec{p}})^2}\,, \tag{4.14}$$

where

$$f(\vec{q},E)=\int_0^\infty dE_{\vec{p}}\frac{N(E_{\vec{p}})}{(E-E_{\vec{p}})(E-E_{\vec{p}+\vec{q}})} \tag{4.15}$$

and

$$E_b=-16\pi^2/\beta^2\,. \tag{4.16}$$

The integrals shown above may be calculated exactly, as shown in Appendixes A and B. We then may rewrite Eq. (4.14) as

$$I_1=\frac{2|E_b|^{1/2}}{q}\left[\frac{\pi}{2}-\tan^{-1}\left(\frac{2|E_b|^{1/2}}{q}\right)\right]. \tag{4.17}$$

The evaluation of I_2, the integral around the branch cut, is shown in Appendix C. Its contribution for the induced density $\langle\rho(\vec{q})\rangle$ is transcribed below:

$$I_2=\frac{1}{\beta}P\int_0^\infty dE_{\vec{p}}N(E_{\vec{p}})\times\left(\frac{n(E_{\vec{p}})}{(E_{\vec{p}}-E_{\vec{p}+\vec{q}})[1/\beta^2+\pi^2N^2(E_{\vec{p}})]}+\frac{n(E_{\vec{p}+\vec{q}})}{(E_{\vec{p}+\vec{q}}-E_{\vec{p}})[1/\beta^2+\pi^2N^2(E_{\vec{p}+\vec{q}})]}\right), \tag{4.18}$$

where $n(E_{\vec{p}})=1$ for $E_{\vec{p}}<E_{\vec{p}_F}$ and $n(E_{\vec{p}})=0$ for $E_{\vec{p}}>E_{\vec{p}_F}$ were introduced to avoid an explicit restriction on the region of $E_{\vec{p}}$-integration.

We now examine in detail the induced density of Fermi particles due to the δ attractive potential as a function of the renormalized potential β.

A. Case I: $1/\beta$ large, $1/\beta^2\gg\pi^2N^2(E_F)$

a. $1/\beta>0$

$$\langle\rho(\vec{q})\rangle=\frac{32\pi^2f(\vec{q},E_b)}{\beta}=\frac{8\pi}{q\beta}\left[\frac{\pi}{2}-\tan^{-1}\left(\frac{8\pi}{q\beta}\right)\right]. \tag{4.19}$$

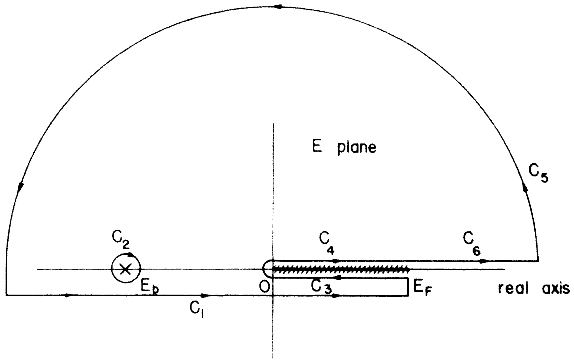

FIG. 3. Contour for evaluation of $\langle\rho(\vec{q})\rangle$ given by Eq. (4.13).

Only the bound state contributes to the particle-density enhancement, the other contributions being of higher order. For large q's, $\langle\rho(\vec{q})\rangle$ goes as $1/q$, leading to a divergence of the particle density around the impurity of the form $1/r^2$. This limit result is the same as that obtained in Sec. II for the one-particle problem.

In this case,

$$g(\vec{r})-1=\frac{|\psi(\vec{r})|^2}{\rho_0}=\frac{|E_b|^{1/2}}{2\pi\rho_0r^2}e^{-2|E_b|^{1/2}r} \tag{4.20}$$

and

$$\int d\vec{r}\,\rho_0[g(\vec{r})-1]=1\,, \tag{4.21}$$

this being the contribution of the bound particle.

b. $1/\beta<0$

$$\langle\rho(\vec{q})\rangle=\beta\chi_0(\vec{q},0)=\beta P\int_0^\infty dE_{\vec{p}}N(E_{\vec{p}})\frac{n(E_{\vec{p}})-n(E_{\vec{p}+\vec{q}})}{E_{\vec{p}}-E_{\vec{p}+\vec{q}}}\,. \tag{4.22}$$

Singwi's result[2] is obtained in this case up to terms of the order β^3. The divergence of $g(\vec{r})$, for $r\to0$, is of the form $1/r$. The plot of $g(\vec{r})$, for $r_s=4$, is shown in Fig. 2. Only scattering states are important and Singwi's theory is exact to first order in β.

B. Case II: $1/\beta$ small, $1/\beta^2\ll\pi^2N^2(E_F)$

a. $1/\beta>0$

$$\langle\rho(\vec{q})\rangle=\frac{8\pi}{q\beta}\left[\frac{\pi}{2}-\tan^{-1}\left(\frac{8\pi}{q\beta}\right)\right]+\frac{2}{\beta\pi^2}P\int_{-\infty}^\infty dE_{\vec{p}}\frac{n(E_{\vec{p}})}{N(E_{\vec{p}})}\frac{1}{E_{\vec{p}}-E_{\vec{p}+\vec{q}}} \tag{4.23}$$

or, performing the integration,

$$\langle\rho(\vec{q})\rangle=\frac{8\pi}{q\beta}\left\{\left[\frac{\pi}{2}-\tan^{-1}\left(\frac{8\pi}{q\beta}\right)\right]+\frac{1}{2\pi}\int_0^{2q_F/q}dx\frac{1}{x}\ln\left|\frac{1+x}{1-x}\right|\right\}. \tag{4.24}$$

There are now two contributions to $g(\vec{r})$, one due to the bound state and another due to scattering states. Both are of the same order β^{-1}. The bound-state contribution is of the same form as case Ia, but the scattering contribution is different from that in Singwi's theory.[2] The difference is due to the fact that in case I the T matrix is essentially independent of the scattered-wave energies, while in case II the effective T matrix is energy dependent and thus the simple effective-potential approximation is no longer valid. $g(\vec{r})$ shows a combined behavior, the bound-state contribution predominant for small r's, going as $1/r^2$; the scattering-wave contribution goes as $1/r$ in this limit (see Fig. 4).

b. $1/\beta < 0$

$$\langle \rho(\vec{q}) \rangle = \frac{-4}{q\beta} \int_0^{2q_F/q} dx \frac{1}{x} \ln \left| \frac{1+x}{1-x} \right| . \tag{4.25}$$

The same comments as those in case II*a* apply here, the bound-state contribution being subtracted off.

V. DISCUSSION AND COMPARISON OF THE RESULTS: CASE OF INTERACTING PARTICLES

We now summarize the results found in the previous sections. The self-consistent approach of Singwi *et al.* does not take into account bound states for the potential chosen in this paper. We believe this to be true and extendable for any potential. The self-consistent approach is correct for a range of energies where the T matrix is approximately energy independent. For an energy-dependent T matrix their result is only qualitatively correct.

One might expect that the particle-particle interaction would minimize the imperfections of the theory and help in preventing the formation of a bound state. We believe, nevertheless, that our conclusions would still be the same and, in the case of a δ potential, the replacement of $\phi(\vec{q}) = \beta$ by

$$\bar{\phi}(\vec{q}) = \beta / \epsilon(\vec{q}) \tag{5.1}$$

does not affect essentially our results.

We could start, from the beginning, with the shielded potential $\bar{\phi}(\vec{q})$ but this procedure, in our point of view, would only complicate the calculations and obscure the interpretations. The correct $\epsilon(\vec{q})$ would, by the way, be the particle–test-charge dielectric function, which in Singwi's theory is given by

$$\epsilon(\vec{q}, 0) = 1 - \psi(\vec{q}) \chi_0(\vec{q}, 0) , \tag{5.2}$$

where $\psi(\vec{q})$ is given by Eq. (3.5). The form and properties of this dielectric function are discussed elsewhere.[9]

The problem of the already mentioned anomalous enhancement of the positron annihilation rate for a low-density electron gas may be due to the inapplicability of the self-consistent approach for such densities.

An anomalous result is also obtained by Sjölander and Stott in the case of an attractive Coulomb interaction between an infinitely heavy impurity and the electron gas. Again a bound state or energy-dependent effective potentials may be responsible for the incorrect results.

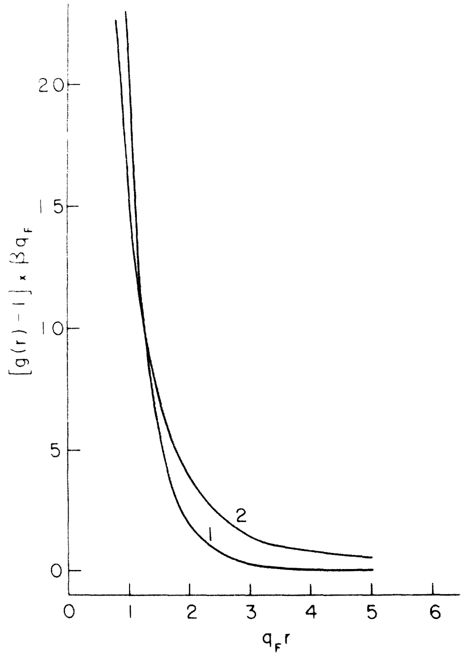

FIG. 4. $[g(r) - 1]\beta q_F$ vs $q_F r$. Curve 1 is the bound-state contribution calculated for $\beta q_F = 8\pi$ and curve 2 is the scattering-state contribution.

VI. CONCLUSIONS

In this paper we studied a δ-function attractive potential embedded in a Fermi gas. We compared the exact results obtained from a Green's-function calculation with those obtained for a free particle and for a Fermi gas in the SCA. The range of validity of the SCA was analyzed, the conclusion being that no bound-state contribution is included in the SCA and that its validity is restricted to a range where the effective potential is essentially energy independent.

We conclude that, if our treatment may be extended for other potentials, the SCA is correct whenever the system is far away from a bound state and, better yet, for large and repulsive potentials. We have shown, moreover, that it is not permissible to add the SCA result and the bound state one since for the region where both occur the T matrix is energy dependent and the SCA fails.

APPENDIX A: DETERMINATION OF E_b

For $\beta > 0$, the integral given by Eq. (4.12) has one pole corresponding to a negative real E. The energy at the pole, E_b, is determined by the equation

$$\frac{1}{\beta}=\int dE_{\vec{p}}\,\frac{E_b N(E_{\vec{p}})}{E_{\vec{p}}(E_b-E_{\vec{p}})}\,, \tag{A1}$$

where

$$N(E_{\vec{p}})=(1/4\pi^2)\,|E_{\vec{p}}|^{1/2} \tag{A2}$$

is the density of states for spinless particles.

Substituting $N(E_{\vec{p}})$ into Eq. (A1) the integral can be evaluated straightforwardly leading to the following expression for E_b:

$$E_b=-16\pi^2/\beta^2\,. \tag{A3}$$

APPENDIX B: EXACT CALCULATION OF $f(\vec{q},E_b)$

We are interested in obtaining the solution of the integral given by Eq. (4.15), for $E=E_b$, which is

$$f(\vec{q},E_b)=\int_0^\infty dE_{\vec{p}}\,\frac{N(E_{\vec{p}})}{(E_b-E_{\vec{p}})(E_b-E_{\vec{p}+\vec{q}})}\,. \tag{B1}$$

This equation can be rewritten in terms of $\vec{p}$ and $\vec{q}$ as

$$f(\vec{q},E_b)=\int\frac{d\vec{p}}{(2\pi)^3}\,\frac{1}{(E_b-p^2)[E_b-(\vec{p}+\vec{q})^2]}\,. \tag{B2}$$

Performing the angular integration in Eq. (B2) and noting that the integrand is an even function of p, that equation reduces to the expression

$$f(\vec{q},E_b)=\frac{1}{16\pi^2 q}\int_{-\infty}^{\infty}dp\,\frac{p}{(|E_b|+p^2)}\ln\frac{|E_b|+(p-q)^2}{|E_b|+(p+q)^2}\,. \tag{B3}$$

We can obtain a considerable simplification if we use the following equivalence:

$$\int_{-\infty}^{\infty}dx\,\frac{x}{1+x^2}\ln[1+(x-y)^2]=\int_{-\infty}^{\infty}dx\,\frac{x}{1+x^2}\ln[1+(x+y)^2]\,, \tag{B4}$$

which is easily verified by an integration by parts. Then, using this relation, we write Eq. (B3) as

$$f(\vec{q},E_b)=(1/8\pi^2 q)I(\vec{q},E_b)\,, \tag{B5}$$

where

$$I(\vec{q},E_b)=\int_{-\infty}^{\infty}dp\,\frac{p}{(|E_b|+p^2)}\ln[|E_b|+(p-q)^2]\,. \tag{B6}$$

To compute this integral we firstly take the q derivative $I'(\vec{q},E_b)$ of $I(\vec{q},E_b)$ which we find to be

$$I'(\vec{q},E_b)=\int_{-\infty}^{\infty}dp\,\frac{-2p(p-q)}{(|E_b|+p^2)[|E_b|+(p-q)^2]}\,. \tag{B7}$$

The integral can be easily performed by residues, by closing the contour on the upper half of the complex plane encircling the poles $i|E_b|^{1/2}$ and $q+i|E_b|^{1/2}$. We obtain the result

$$I'(\vec{q},E_b)=\frac{-4\pi|E_b|}{4|E_b|+q^2}\,. \tag{B8}$$

To determine $I(\vec{q},E_b)$ we integrate Eq. (B8) with $I(0,E_b)=0$. We obtain

$$I(\vec{q},E_b)=2\pi\tan^{-1}(2|E_b|^{1/2}/q)-\pi^2\,. \tag{B9}$$

Finally we write Eq. (B5) as

$$f(\vec{q},E_b)=\frac{1}{4\pi q}\left(\tan^{-1}\frac{2|E_b|^{1/2}}{q}-\frac{\pi}{2}\right). \tag{B10}$$

APPENDIX C: DETERMINATION OF I_2

We want to find I_2, the E integral of $\delta\tilde{G}(\vec{q},E)$ along the curves C_3 and C_4 shown in Fig. 3. I_2 is given by

$$I_2=-i\int_0^{E_F}\frac{dE}{2\pi}\,[\delta\tilde{G}(\vec{q},E)-\delta\tilde{G}^*(\vec{q},E)]\,, \tag{C1}$$

where $\delta\tilde{G}(\vec{q},E)$, for complex E, is given by

$$\delta\tilde{G}(\vec{q},E)=\int_0^\infty dE_{\vec{p}}\,\frac{N(E_{\vec{p}})}{E-E_{\vec{p}}+i\eta_{\vec{p}}}\,\frac{1}{E-E_{\vec{p}+\vec{q}}+i\eta_{\vec{p}+\vec{q}}}\times\left(\frac{1}{\beta}-\int dE_{\vec{p}}\,\frac{EN(E_{\vec{p}})}{E_{\vec{p}}(E-E_{\vec{p}}-i\eta)}\right)^{-1} \tag{C2}$$

and $\delta\tilde{G}^*(\vec{q},E)$ is its complex conjugated.

Inserting Eq. (C2) into Eq. (C1) we obtain

$$I_2=-i\int_0^{E_F}\frac{dE}{2\pi}\int_0^{E_F}dE_{\vec{p}}\,2i\times\mathrm{Im}\left(\frac{N(E_{\vec{p}})}{E-E_{\vec{p}}+i\eta_{\vec{p}}}\,\frac{1}{E-E_{\vec{p}+\vec{q}}+i\eta_{\vec{p}+\vec{q}}}\times\frac{1}{1/\beta-P(E)-i\pi N(E)}\right), \tag{C3}$$

where

$$P(E)=P\int dE_{\vec{p}}\,\frac{EN(E_{\vec{p}})}{E_{\vec{p}}(E-E_{\vec{p}})}\,, \tag{C4}$$

P meaning the principal part of the integral. We can verify that the solution of this last integral goes to zero for $E>0$.

Then, performing the E integral in Eq. (C3), we obtain

$$I_2 = P\int_0^{E_F} dE_{\vec p}\, N(E_{\vec p}) \left(\frac{1}{E_{\vec p}-E_{\vec p+\vec q}}\, \frac{1/\beta}{1/\beta^2+\pi^2N^2(E_{\vec p})} + \frac{1}{E_{\vec p+\vec q}-E_{\vec p}}\, \frac{1/\beta}{1/\beta^2+\pi^2N^2(E_{\vec p+\vec q})} + \int_0^{E_F} dE\, \frac{N(E)}{(E-E_{\vec p})(E-E_{\vec p+\vec q})}\, \frac{1}{1/\beta^2+\pi^2N^2(E)} \right). \tag{C5}$$

We now rewrite Eq. (C5) as

$$I_2 = \frac{1}{\beta} P\int_0^{\infty} dE_{\vec p}\, N(E_{\vec p}) \left(\frac{n(E_{\vec p})}{(E_{\vec p}-E_{\vec p+\vec q})[1/\beta^2+\pi^2N^2(E_{\vec p})]} + \frac{n(E_{\vec p+\vec q})}{(E_{\vec p+\vec q}-E_{\vec p})[1/\beta^2+\pi^2N^2(E_{\vec p+\vec q})]} \right) + P\int_0^{\infty} dE_{\vec p}\, N(E_{\vec p}) \int_0^{E_F} dE\, \frac{N(E)}{(E-E_{\vec p})(E-E_{\vec p+\vec q})}\, \frac{1}{[1/\beta^2+\pi^2N^2(E)]}\,. \tag{C6}$$

Next, we calculate the last $E_{\vec p}$ integral in Eq. (C6) using residue theory. Since the integrand is an analytic function of $E_{\vec p}$ except on the real axis the principal part of the integral goes to zero and Eq. (C6) can be rewritten in the form

$$I_2 = \frac{1}{\beta} P\int_0^{\infty} dE_{\vec p}\, N(E_{\vec p}) \left(\frac{n(E_{\vec p})}{(E_{\vec p}-E_{\vec p+\vec q})[1/\beta^2+\pi^2N^2(E_{\vec p})]} + \frac{n(E_{\vec p+\vec q})}{(E_{\vec p+\vec q}-E_{\vec p})[1/\beta^2+\pi^2N^2(E_{\vec p+\vec q})]} \right). \tag{C7}$$

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*Work supported by BNDE, CAPES, CNPq, and FAPESP.

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