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Approximate Screening Functions in Metals*

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A variational principle is used to "solve" an approximate integral equation for the screening functions of the electron gas. It is shown that the simplest possible trial function gives a solution to the equation for the dielectric constant which is exact in both the limits of small and large momentum transfers. The results are compared with other calculations. It is shown that the approximation developed recently by Kleinman is quite good in the static large-k limit, but otherwise incorrect. The dielectric constant derived from the variational calculation is used to derive an expression for the ground-state energy; this expression is similar in its essential features to the interpolation schemes of Hubbard and of Nozières and Pines, even though the Hubbard approximation considerably underestimates the exchange enhancement of the vertex function at large k. Finally, it is suggested that similar variational principles may have other uses, as in the paramagnon problem.

I. INTRODUCTION

A KNOWLEDGE of the linear response of an electron gas, to external perturbations, aside from its intrinsic interest, is an essential ingredient in a large class of calculations in free-electron-like metals. Of particular interest is the inverse dielectric constant $\epsilon^{-1}(k)$, which gives the electric potential surrounding a unit external potential, and the vertex function $\Lambda_k(p)$, which gives the matrix element for the scattering of an electron by a unit external potential from an initial state p to a final state $p+k$, where $k=(\mathbf{k},\omega)$ and $p=(\mathbf{p},\Omega)$. The static ($\omega=0$) values of these functions are needed for calculations of band structure, thermal and transport coefficients, and phonon spectra, while the full frequency-dependent values shed light on collective oscillations, optical transitions, excitons, and possible charge-density wave instabilities.

Despite their importance, however, ϵ and Λ are not well known at metallic densities except in a few limits.

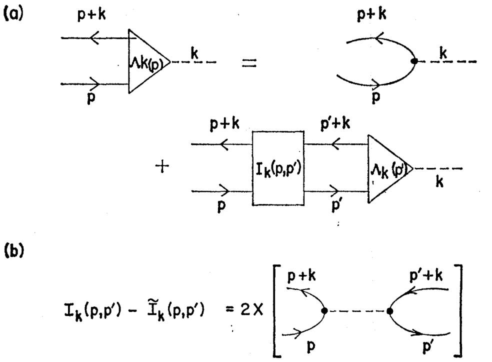

FIG. 1. In (a) is shown the diagrammatic representation of Eq. (1). It also gives the diagrammatic representation of Eq. (3) provided that I and Λ are replaced by $\tilde{I}$ and $\tilde{\Lambda}$, respectively. In (b) is shown the relationship between I and $\tilde{I}$; the factor of 2 arises from the spin summation over the primed variables. The internal lines on (a) and (b) represent the propagator G. The external lines are shown for clarity, but are not included in the definitions of I and Λ.

To calculate Λ, one must solve the equation

$$\Lambda_k(p)=1+\int_{p'} I_k(p,p')G(p')G(p'+k)\Lambda_k(p'), \qquad (1)$$

where G is the propagator for an electron in the state p, and $I_k(p,p')$ is the spin symmetric part of the effective particle-hole interaction. The notation $\int_{p'}$ is the abbreviation for

$$\int\frac{d^3p'}{(2\pi)^3}\int\frac{d\Omega'}{2\pi i}.$$

In terms of Λ, the dielectric function is given by

$$\frac{1}{\epsilon(k)}-1=2V_k\int_{p'}\Lambda_k(p')G(p')G(p'+k), \qquad (2)$$

where V_k is the Coulomb matrix element $4\pi e^2/k^2$. Generally, (1) is simplified by separating out the singular direct Coulomb part of I, letting $I_k(p,p')=\tilde{I}_k(p,p')+2V_k$ and $\tilde{\Lambda}_k(p)=\epsilon(k)\Lambda_k(p)$. Then (1) and (2), respectively, become

$$\tilde{\Lambda}_k(p)=1+\int_{p'}\tilde{I}_k(p,p')G(p')G(p'+k)\tilde{\Lambda}_k(p') \qquad (3)$$

and

$$\epsilon(k)-1=-2V_k\int_{p'}\tilde{\Lambda}_k(p')G(p')G(p'+k). \qquad (4)$$

Equations (1)–(4), which are derived in the standard textbooks,[1] are illustrated graphically in Fig. 1.

The difficulty in finding $\tilde{\Lambda}$ involves not only solving the integral equation (3), but also in determining $\tilde{I}$ which is itself unknown. Previous work has been reviewed by Geldhart and Vosko,[2] who emphasize the importance of making self-consistent (Φ derivable, in

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[1] P. Nozières, *Theory of Interacting Fermi Systems* (W. A. Benjamin, Inc., New York, 1954); A. A. Abrikosov, L. P. Gor'kov, and I. E. Dzyaloshinski, *Methods of Quantum Field Theory in Statistical Physica* (Prentice-Hall, Inc., Englewood Cliffs, N. J., 1963).

[2] D. J. W. Geldart and S. H. Vosko, Can. J. Phys. 44, 2137 (1966).

sense of Baym[3]) approximations. The difficulty in finding $\tilde{\Lambda}$ is compounded by the fact that $\tilde{I}$ is frequency-dependent as well as momentum-dependent. This is especially important for small momentum transfer k, where neglect of the frequency dependence will result in an error in $\tilde{\Lambda}$ by a factor $\sim Z$ (the wave-function renormalization factor), even if the effective mass and compressibility are given accurately; according to Rice's calculations,[4] Z can differ considerably from unity at metallic densities. On the other hand, perhaps these small-k difficulties are not so serious, at least for $\omega=0$, because Λ and ϵ are given by Ward identities[5]

$$\begin{aligned}\Lambda^{-1} &\rightarrow 1+(m^*/m)Z(k_{\mathrm{FT}}^2/k^2),\\ \epsilon &\rightarrow 1+(k_{\mathrm{FT}}^2/k^2)(\kappa/\kappa_0),\end{aligned} \tag{5}$$

where κ/κ_0 is the compressibility enhancement due to electron-electron interactions, m^* is the effective mass, and k_{FT} is the inverse Fermi-Thomas length. The quantities κ and m^* in turn may be calculated with some degree of confidence using the interpolation procedures developed by Nozières and Pines,[6] Hubbard,[7] and others.[8]

One common approximation, first exploited by Hubbard,[7] and used by many others since, was to replace $\tilde{I}$ by a static interaction

$$\tilde{I}(\mathbf{p},\mathbf{p}')=-\{4\pi e^2/[(\mathbf{p}-\mathbf{p}')^2+K_s^2]\}, \tag{6}$$

where K_s was a screening parameter, usually taken to be the inverse Fermi-Thomas length.[9] As $k\rightarrow 0$, such a static approximation can only be viable at metallic densities if (3) is regarded as an equation for the physical quantity $Z\tilde{\Lambda}_{k,0}$ rather than $\tilde{\Lambda}_{k,0}$ itself, because then the most important effect of a dynamic interaction (the appearance of Z) cancels out according to (5). At finite k, one would then assume that the same cancellation still occurs, at least approximately.[10] For very large k, on the other hand, frequency-dependent effects presumably become less important. In any case, Eq. (6) becomes essentially a definition rather than an approximation if K_s^2 is regarded as a complex function of all the variables; it will be a useful definition if it turns out that the various calculated quantities are not very sensitive to the value of K_s^2. According to our later estimates, this is roughly true at large k (assuming that we have reasonably guessed the size of K_s^2).

The assumption of a static interaction leads to considerable simplification, and (3) and (4) become

$$\tilde{\Lambda}_{\mathbf{k}\omega}(\mathbf{p})=1-\sum_{\mathbf{p}'}\tilde{I}(\mathbf{p},\mathbf{p}')g_{\mathbf{k}\omega}(\mathbf{p}')\tilde{\Lambda}_{\mathbf{k}\omega}(\mathbf{p}') \tag{7}$$

and

$$\epsilon(\mathbf{k},\omega)=1+2V_{\mathbf{k}}\sum_{\mathbf{p}'}g_{\mathbf{k}\omega}(\mathbf{p}')\tilde{\Lambda}_{\mathbf{k}\omega}(\mathbf{p}'), \tag{8}$$

where

$$g_{\mathbf{k}\omega}(\mathbf{p})=(f_{\mathbf{p}+\mathbf{k}}-f_{\mathbf{p}})/(\omega+i\eta+\epsilon_{\mathbf{p}}-\epsilon_{\mathbf{p}+\mathbf{k}}), \tag{9}$$

where $\epsilon_p=p^2/2m+\sum_{\mathbf{p}'}\tilde{I}(\mathbf{p},\mathbf{p}')f_{\mathbf{p}'}$, η is a positive infinitesimal,[11] $f_{\mathbf{p}}$ is the Fermi function, and $\sum_p$ is shorthand for $(2\pi)^{-3}\int d^3p$. Hubbard then solved (7) approximately by assuming that $(\mathbf{p}-\mathbf{p}')^2$ could be replaced by $k^2+k_{\mathrm{F}}^2$ (k_{F}=the Fermi wave number), so that $\tilde{\Lambda}_{\mathbf{p}\omega}(\mathbf{p})$ was independent of $\mathbf{p}$ and given by

$$\tilde{\Lambda}_{\mathbf{k}\omega}(\mathbf{p})=[1+\langle\tilde{I}\rangle\Pi^{(0)}(\mathbf{k}\omega)]^{-1}, \tag{10}$$

where

$$\langle\tilde{I}\rangle=-[4\pi e^2/(k^2+k_{\mathrm{F}}^2+K_s^2)] \tag{11}$$

and $\Pi^{(0)}(\mathbf{k}\omega)=\sum_{\mathbf{p}}g_{\mathbf{k}\omega}(\mathbf{p})$ is the polarization propagator of the noninteracting electron gas, first evaluated by Lindhard.[12] The corresponding approximations for ϵ and Λ are

$$\epsilon(\mathbf{k},\omega)=1+2V_k\Pi^{(0)}(\mathbf{k}\omega)[1+\langle\tilde{I}\rangle\Pi^{(0)}(\mathbf{k}\omega)]^{-1} \tag{12a}$$

[using (8) and (10)] and

$$\Lambda_{\mathbf{k}\omega}=[1+(2V_k+\langle\tilde{I}\rangle)\Pi^{(0)}(\mathbf{k}\omega)]^{-1} \tag{12b}$$

[using $\tilde{\Lambda}=\epsilon\Lambda$]. Hubbard[7] originally used (12) to calculate the ground-state energy of an electron gas, but since then, many others have applied it in calculations of other metallic properties.

Recently, however, it was suggested independently by Kleinman[13] and Overhauser[14] that the $\mathbf{k}$ dependence of (11) at large k is completely incorrect. Both authors, in effect, solved (7) approximately with an interaction similar to (6), finding a vertex function of the form (10) (at least for $\omega=0$), but with $\langle\tilde{I}\rangle$ having a different form from (11). These assertions, if true, could have large effects on the properties of the electron gas; in particular, the correlation energy at metallic densities is sensitive to the large-k dependence of (12); could it be that the hitherto believed most reliable calculations of the correlation energy are incorrect?

Because the connection between Kleinman's and Overhauser's treatments and the more conventional formulations is far from clear, we begin by briefly discussing their calculations. In particular, Overhauser's

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[3] G. Baym, Phys. Rev. **127**, 1391 (1962).

[4] T. M. Rice, Ann. Phys. (N. Y.) **31**, 100 (1965).

[5] J. M. Luttinger and P. Nozières, Phys. Rev. **127**, 1423 (1962); **127**, 1431 (1962).

[6] P. Nozières and D. Pines, Phys. Rev. **111**, 442 (1958).

[7] J. Hubbard, Proc. Roy. Soc. (London) **A243**, 336 (1957).

[8] See D. Pines and P. Nozières, *Theory of Quantum Liquids* (W. A. Benjamin, Inc., New York, 1966), Vol. I.

[9] The screening was not added until later. See L. J. Sham, Proc. Roy. Soc. (London) **283**, 33 (1965); S. H. Vosko, R. Taylor, and G. H. Keech, Can. J. Phys. **43**, 1187 (1965); V. Heine and I. Abarenkov, Phil. Mag. **9**, 451 (1964); L. M. Falicov and V. Heine, Advan. Phys. **10**, 57 (1961).

[10] At finite but small k and finite ω, this cancellation would not still occur, even though as $k\rightarrow 0$, ω finite Eq. (6) gives an $\epsilon(\mathbf{k}\omega)$ which is exact.

[11] Having already performed all frequency integrations, we have no further use for the analytic structure of the time-ordered product, and thus have switched to the physically meaningful analytic structure of the retarded commutator.

[12] J. Lindhard, Kgl. Danske Videnskab. Selskab, Mat.-Fys. Medd. **28**, 8 (1954).

[13] L. Kleinman, Phys. Rev. **160**, 585 (1967). The more recent calculation of Kleinman's [Phys. Rev. **172**, 393 (1968)] appeared after this manuscript was completed, and will not be discussed here.

[14] A. W. Overhauser, Phys. Rev. **156**, 844 (1967).

work is outwardly a calculation of the optical properties of free-electron-like metals. We show that the calculated modification in the strength of the absorption results from a final-state interaction due to the existence of an exciton state, manifested by a zero in $\epsilon(\mathbf{k},\omega)$. Since this zero exists even at $\omega=0$ for finite $\mathbf{k}$, the ground state would be unstable to the formation of static charge-density fluctuations if Overhauser's calculation is correct.

In Sec. IV, we develop a variational principle to solve (7). Using the simplest possible trial solution, we find that the resulting expression for ϵ using (8) is exact in both the large-k and small-$\mathbf{k}$ limits, and provides an interpolation for intermediate values, regardless of the form chosen for $\tilde{I}(\mathbf{p},\mathbf{p}')$. Taking $\tilde{I}$ to be given by (6), we find that Kleinman's approximation (for $\omega=0$) is quite accurate for large $\mathbf{k}$, but gets worse as $\mathbf{k}$ decreases. Kleinman's frequency-dependent results, however, are incorrect and we suggest the appropriate modifications. If we force our results into the form (10), defining an effective $\langle\tilde{I}\rangle$ (now a complex function of $\mathbf{k}$ and ω), we find that $\langle\tilde{I}\rangle$ is not very sensitive to the value of the screening parameter K_s for large k, except for very small K_s. From this we conclude that (i) to the extent that the evils of the static approximation (6) can be absorbed into a renormalized screening parameter, their effect is relatively slight and (ii) only a small amount of screening is necessary to destroy the exciton (charge-density fluctuation) instability of Overhauser.

In any case the k dependence of $\langle\tilde{I}\rangle$ (at large $\mathbf{k}$) proposed by Kleinman and Overhauser is correct. This leaves the question raised earlier about the correlation energy. To answer it we perform the usual frequency and coupling constant integration of ϵ^{-1}, taking ϵ from our variational calculation. The result is that the coefficients of the anomalously $\mathbf{k}$-dependent terms integrate to zero, and we are left with an expression for the correlation energy which in its essential features is identical to those proposed by Nozières and Pines,[6] and Hubbard.[7]

II. KLEINMAN'S CALCULATION

Kleinman calculates Λ in the Hartree-Fock approximation and later includes the effects of correlation phenominologically. We show here that his approximation is tantamount to Eqs. (6) and (7). We do this mainly to make contact with his notation and to see where his approximations enter, since it is obvious by inspection that the Hartree-Fock approximation[15] consists in letting $\tilde{I}(\mathbf{p},\mathbf{p}')=-4\pi e^2/(\mathbf{p}-\mathbf{p}')^2$ in (7), with ϵ_p given in Ref. 10.

Essentially, one applies an external potential V^{ext}, and calculates the induced one-electron Hartree-Fock potential V^{HF} self-consistently in lowest-order perturbation theory, that is,

$$V^{\mathrm{HF}}=V^{\mathrm{ext}}+V^{\mathrm{Coul}}+V^{\mathrm{exch}}, \qquad (13)$$

where V^{Coul} and V^{exch} are, respectively, the direct Coulomb and exchange terms of the Hartree-Fock equation. For simplicity, one takes V^{ext} only to have matrix elements between plane-wave states $\mathbf{p}$ and $\mathbf{p}'$ separated by momentum transfer $\mathbf{k}$, so that V^{HF}, V^{Coul}, and V^{exch} will also have this property. Thus we write

$$\langle\mathbf{p}'|V|\mathbf{p}\rangle=V_{\mathbf{k}}(\mathbf{p},t)\delta_{\mathbf{p}',\mathbf{p}+\mathbf{k}}+V_{-\mathbf{k}}(\mathbf{p},t)\delta_{\mathbf{p}',\mathbf{p}-\mathbf{k}}, \qquad (14)$$

with

$$V_{\mathbf{k}}(\mathbf{p},t)=[V_{\mathbf{k},\omega}(\mathbf{p})e^{-i\omega t}+V_{\mathbf{k},-\omega}(\mathbf{p})e^{i\omega t}]e^{\eta t}, \qquad (15)$$

where V can have any superscript ("HF," "Coul," "exch," or "ext"). Since V is Hermitian, we note that

$$V_{\mathbf{k},\omega}(\mathbf{p})=[V_{-\mathbf{k},-\omega}(\mathbf{p}+\mathbf{k})]^*. \qquad (16)$$

Also, in terms of (14) and (15), we may write the vertex and dielectric functions[16] as

$$V_{\mathbf{k}\omega}{}^{\mathrm{HF}}(\mathbf{p})=\Lambda_{\mathbf{k}\omega}(\mathbf{p})V_{\mathbf{k}\omega}{}^{\mathrm{ext}}(\mathbf{p}) \qquad (17)$$

and

$$V_{\mathbf{k}\omega}{}^{\mathrm{Coul}}(\mathbf{p})=[\epsilon^{-1}(\mathbf{k},\omega)-1]V_{\mathbf{k}\omega}{}^{\mathrm{ext}}(\mathbf{p}). \qquad (18)$$

According to time-dependent perturbation theory, the single-particle wave function is

$$\begin{aligned}\phi_{\mathbf{p}'}(\mathbf{r})=e^{-i\epsilon_{p'}t}\{e^{i\mathbf{p}'\cdot\mathbf{r}}&+[a_{\mathbf{k},\omega}(\mathbf{p}')+a_{\mathbf{k},-\omega}(\mathbf{p}')]e^{i(\mathbf{p}'+\mathbf{k})\cdot\mathbf{r}}\\&+[a_{-\mathbf{k}\omega}(\mathbf{p}')+a_{\mathbf{k},-\omega}(\mathbf{p}')]e^{i(\mathbf{p}'-\mathbf{k})\cdot\mathbf{r}}\}, \qquad (19)\end{aligned}$$

where[17]

$$a_{\mathbf{k}\omega}(\mathbf{p}')=[V_{\mathbf{k}\omega}{}^{\mathrm{HF}}(\mathbf{p}')e^{-i\omega t}/(\omega+i\eta+\epsilon_{p'}-\epsilon_{\mathbf{p}'+\mathbf{k}})]. \qquad (20)$$

By calculating the Coulomb matrix element

$$\begin{aligned}\langle\mathbf{p}+\mathbf{k}|V^{\mathrm{Coul}}|\mathbf{p}\rangle=2\sum_{p'<k_{\mathrm{F}}}\int d^3r_1\int d^3r_2\\ \times e^{-i(\mathbf{p}+\mathbf{k})\cdot\mathbf{r}_1}\phi_{p'}{}^*(\mathbf{r}_2)\frac{e^2}{|\mathbf{r}_1-\mathbf{r}_2|}\phi_{p'}(\mathbf{r}_2)e^{i\mathbf{p}\cdot\mathbf{r}_1}, \qquad (21)\end{aligned}$$

and comparing with (14) and (15), one obtains[18]

$$V_{\mathbf{k}\omega}{}^{\mathrm{Coul}}(\mathbf{p})e^{i\omega t}=2V_{\mathbf{k}}\sum_{\mathbf{p}'}f_{p'}[a_{\mathbf{k}\omega}(\mathbf{p}')+a_{-\mathbf{k},-\omega}{}^*(\mathbf{p}')]. \qquad (22)$$

Similarly, by calculating

$$\begin{aligned}\langle\mathbf{p}+\mathbf{k}|V^{\mathrm{exch}}|\mathbf{p}\rangle=-\sum_{\mathbf{p}'}f_{p'}\int d^3r_1\int d^3r_2\\ \times e^{-(\mathbf{p}+\mathbf{k})\cdot\mathbf{r}_1}\phi_{p'}(\mathbf{r}_2)\frac{e^2}{|\mathbf{r}_1-\mathbf{r}_2|}\phi_{p'}(\mathbf{r}_1)e^{i\mathbf{p}\cdot\mathbf{r}_2}, \qquad (23)\end{aligned}$$

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[15] Also called the generalized random-phase approximation; see Ref. 8, p. 317ff.

[16] To obtain Kleinman's notation and units from ours, make the replacements $\epsilon\to\epsilon_t$, $\Lambda^{-1}\to\epsilon_e$, $\omega\to-\omega$, $\mathbf{k}\to\boldsymbol{\kappa}$, $\mathbf{p}\to\mathbf{k}$, $e^2\to2$, $2m\to1$.

[17] $V_{\mathbf{k}\omega}{}^{\mathrm{HF}}(\mathbf{p}')$ is the analog of Kleinman's $V_{\mathbf{k}\omega\mathbf{p}'}{}^{(+)}$ and $V_{\mathbf{k},-\omega}{}^{\mathrm{HF}}(\mathbf{p}')$ of $V_{\mathbf{k}\omega\mathbf{p}'}{}^{(-)}$. Kleinman's notation seems to imply that he has assumed that $V_{\mathbf{k}\omega}{}^{\mathrm{HF}}(\mathbf{p}')=V_{-\mathbf{k},\omega}{}^{\mathrm{HF}}(\mathbf{p}')$, but this is not true in the general case, even if the external potentials have this property by construction. Equation (20) is the analog of Kleinman's four equations (9).

[18] As implied by our notation, the values of $V_{\mathbf{k},-\omega}$ in Eqs. (22) and (24) are obtained by replacing ω with $-\omega$, and similarly for $\mathbf{k}$.

one finds that[18]

$$V_{\mathbf{k}\omega}{}^{\mathrm{exch}}(\mathbf{p})e^{i\omega t}=-\sum_{\mathbf{p}'}\left[\frac{4\pi e^2}{(\mathbf{p}-\mathbf{p}')^2}a_{\mathbf{k}}(\mathbf{p}')+\frac{4\pi e^2}{(\mathbf{p}+\mathbf{k}-\mathbf{p}')^2}a^*{}_{-\mathbf{k},-\omega}(\mathbf{p}')\right]. \quad (24)$$

Then using (13), (20), (22), and (24), one obtains four[18] equations

$$V_{\mathbf{k}\omega}{}^{\mathrm{HF}}(\mathbf{p})=V_{\mathbf{k}\omega}{}^{\mathrm{ext}}(\mathbf{p})+\frac{8\pi e^2}{k^2}\times\sum_{\mathbf{p}'}f_{p'}\left\{\frac{V_{\mathbf{k}\omega}{}^{\mathrm{HF}}(\mathbf{p}')}{\omega+i\eta+\epsilon_{\mathbf{p}'}-\epsilon_{\mathbf{p}'+\mathbf{k}}}+\frac{[V_{-\mathbf{k},-\omega}{}^{\mathrm{HF}}(\mathbf{p}')]^*}{-\omega-i\eta+\epsilon_{\mathbf{p}'}-\epsilon_{\mathbf{p}'-\mathbf{k}}}\right\}$$
$$-\sum_{\mathbf{p}'}f_{\mathbf{p}'}\left\{\frac{4\pi e^2}{(\mathbf{p}-\mathbf{p}')^2}\frac{V_{\mathbf{k}\omega}{}^{\mathrm{HF}}(\mathbf{p}')}{\omega+i\eta+\epsilon_{\mathbf{p}'}-\epsilon_{\mathbf{p}'+\mathbf{k}}}+\frac{4\pi e^2}{(\mathbf{p}+\mathbf{k}-\mathbf{p}')^2}\times\frac{[V_{-\mathbf{k},-\omega}{}^{\mathrm{HF}}(\mathbf{p}')]^*}{-\omega-i\eta+\epsilon_{\mathbf{p}'}-\epsilon_{\mathbf{p}'-\mathbf{k}}}\right\}. \quad (25)$$

We now note that use of the identity (16) in the square bracketed terms in (25) reduces the four equations (25), to four identical uncoupled equations, the solutions of which satisfy (16). Finally, noting that V^{ext} is independent of **p**, the use of (17) simplifies (25) to

$$\Lambda_{\mathbf{k}\omega}(\mathbf{p})=1-\frac{8\pi e^2}{k^2}\sum_{\mathbf{p}'}g_{\mathbf{k}\omega}(\mathbf{p}')\Lambda_{\mathbf{k}\omega}(\mathbf{p}')+\sum_{\mathbf{p}'}\frac{4\pi e^2}{(\mathbf{p}-\mathbf{p}')^2}g_{\mathbf{k}\omega}(\mathbf{p}')\Lambda_{\mathbf{k}\omega}(\mathbf{p}'), \quad (26)$$

or

$$\tilde{\Lambda}_{\mathbf{k}\omega}(\mathbf{p})=1+\sum_{\mathbf{p}'}\frac{4\pi e^2}{(\mathbf{p}-\mathbf{p}')^2}g_{\mathbf{k}\omega}(\mathbf{p}')\tilde{\Lambda}_{k\omega}(\mathbf{p}'). \quad (27\mathrm{a})$$

We note that Kleinman never used (16), and made the approximation $(\mathbf{p}-\mathbf{p}')^2\simeq k_f{}^2+K_s{}^2$, $(\mathbf{p}+\mathbf{k}-\mathbf{p}')^2\simeq k_f{}^2+K_s{}^2+k^2$ directly in (25). Thus he coupled two equations that are rigorously uncoupled, and his solution fails to satisfy the basic invariance (16). All this is relevant at $\omega=0$, but at finite frequency his results are incorrect.

Equation (27a) makes Kleinman's calculation at $\omega=0$ especially transparent. Substitution of (9) into (27a) yields

$$\tilde{\Lambda}_{\mathbf{k}}(\mathbf{p})=1+\sum_{\mathbf{p}'<k_{\mathrm{F}}}\frac{4\pi e^2}{(\mathbf{p}+\mathbf{k}-\mathbf{p}')^2}\frac{\tilde{\Lambda}_{\mathbf{k}}(\mathbf{p}'-\mathbf{k})}{\epsilon_{\mathbf{p}}-\epsilon_{\mathbf{p}-\mathbf{k}}}-\sum_{\mathbf{p}'<k_{\mathrm{F}}}\frac{4\pi e^2}{(\mathbf{p}-\mathbf{p}')^2}\frac{\tilde{\Lambda}_{\mathbf{k}}(\mathbf{p}')}{\epsilon_{\mathbf{p}}-\epsilon_{\mathbf{p}+\mathbf{k}}} \quad (27\mathrm{b})$$

upon change of the integration variable. Replacement of $(\mathbf{p}+\mathbf{k}-\mathbf{p}')^{-2}$ by $(k^2+k_{\mathrm{F}}{}^2+K_s{}^2)^{-2}$ and $(\mathbf{p}-\mathbf{p}')^{-2}$ by $(k_{\mathrm{F}}{}^2+K_s{}^2)^{-2}$ renders (27b) trivially soluble and Kleinman's expression for $\tilde{\Lambda}$ emerges. Since (27a) was written down by inspection in the Introduction, this constitutes a two-line derivation of Kleinman's results for $\omega=0$.

III. OVERHAUSER'S CALCULATION

Overhauser's calculation was ostensibly one of interband optical absorption in metals. In fact, however, since band-structure effects are treated as weak, his calculation really determines the longitudinal dielectric constant $\epsilon(k,\omega)$ in an approximation similar to Kleinman's. To see this, we note that to lowest order in the bare crystalline potential

$$U(\mathbf{r})=\sum_{\mathbf{G}}U_{\mathbf{G}}e^{i\mathbf{G}\cdot\mathbf{r}},$$

the imaginary part of the optical dielectric constant $\epsilon_2(\omega)$ is given by[19]

$$\epsilon_2(\omega)=(3m^2\omega^4)^{-1}\sum_{\mathbf{G}}|U_{\mathbf{G}}|^2G^4\{-\mathrm{Im}[\epsilon(\mathbf{G},\omega)]^{-1}\}, \quad (28)$$

where **G** is a reciprocal lattice vector. Effectively, then $\epsilon(\mathbf{G},\omega)$ is calculated in the Hartree-Fock approximation, so that ϵ is of the form (12). As in Kleinman's calculation, $\langle\tilde{I}\rangle$ is real and approaches a constant at large k, in contrast with (11). Using (9) and (12) gives

$$-\mathrm{Im}[\epsilon(\mathbf{G},\omega)]^{-1}=|\Lambda_{\mathbf{G},\omega}|^2\frac{4\pi e^2}{G^2}\times\sum_{\mathbf{p}<k_{\mathrm{F}},|\mathbf{p}+\mathbf{G}|>k_{\mathrm{F}}}2\pi\delta(\omega+\epsilon_{\mathbf{p}}-\epsilon_{\mathbf{p}+\mathbf{G}}). \quad (29)$$

On the other hand, the "standard" formula[20] for $\epsilon_2(\omega)$ to lowest order in the potential U is

$$\epsilon_2(\omega)=\frac{4\pi e^2}{3m^2\omega^4}\sum_{\mathbf{G}}|V_{\mathbf{G}}{}^{\mathrm{HF}}|^2G^2\times\sum_{p<k_{\mathrm{F}},|\mathbf{p}+\mathbf{G}|>k_{\mathrm{F}}}2\pi\delta(\omega+\epsilon_{\mathbf{p}}-G_{\mathbf{p}+\mathbf{G}}), \quad (30)$$

where $V_{\mathbf{G}}{}^{\mathrm{HF}}$ is the Hartree-Fock potential used to calculate the band structure, that is $V_{\mathbf{G}}{}^{\mathrm{HF}}=\Lambda_{\mathbf{G},0}U_{\mathbf{G}}$. The ratio of (28) to (30) for a given transition (fixed **G** value) is

$$F_{\mathbf{G}}(\omega)=|\Lambda_{\mathbf{G},\omega}/\Lambda_{\mathbf{G},0}|^2. \quad (31)$$

Comparison with Overhauser's Eq. (17) shows that the $F_{\mathbf{G}}(\omega)$ of (31) is exactly Overhauser's "enhancement" factor. Hence, his calculation is in essence one of the response of an interacting electron gas.

The second point to be made is that for Overhauser's large value of $\langle\tilde{I}\rangle$ ($\simeq 9\pi e^2/k_{\mathrm{F}}{}^2$), the function $F_k(\omega)$ [or $\epsilon^{-1}(\mathbf{k},\omega)$] has a pole in the region $k>2k_{\mathrm{F}}$ and $\omega<(k/m)(\frac{1}{2}k-k_{\mathrm{F}})$. The locus of this pole (ω as a function of k) is sketched in Fig. 2. This pole is the result of his (assumed) strong electron-hole interaction, and

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[19] J. J. Hopfield, Phys. Rev. **139**, A419 (1965).

[20] P. N. Butcher, Proc. Roy. Soc. (London) **A64**, 765 (1951).

represents a particle-hole bound state or exciton. It would show up as an anomalous direct optical transition below the interband threshold in the alkali metals, provided that the 110 reciprocal lattice vector G lies between k_1 and k_2 (see Fig. 2), and might appear as an indirect (phonon-induced transition) otherwise. The anomalous threshold behavior predicted by Overhauser is simply due to the final-state interaction caused by the tendency of electrons and holes to form bound states.

Since there is at least some experimental evidence[21] in the alkalis, not only for anomalous absorption below threshold, but also for anomalous threshold behavior, the above would be an appealing explanation (aside from the theoretical difficulties of manufacturing such a large particle-hole interaction) if it were not for the fact that this exciton state by its very existence implies an instability of the ground state of the electron gas. This is seen most simply by noting that the exciton dispersion relation goes to zero at finite wave vector; since this dispersion relation is determined by the zeros of $\epsilon(k,\omega)$, the electron gas would be unstable toward the formation of static charge-dentisy fluctuations[22] of wave vector $\mathbf{k}$ determined by $\epsilon(\mathbf{k},0)=0$.

IV. VARIATIONAL CALCULATION

The difference between the large-k dependence of $\tilde{\Lambda}$ in the Hubbard approximation, and that given by the methods of Secs. II and III, results only from different approximate solutions of Eq. (7). To solve (7) accurately, we develop a variational principle; we show that the simplest possible trial function gives (8) exactly in both small-k and large-k limits and provides an interpolation for intermediate k.

Although variational principles are commonly used to obtain approximate solutions to the Boltzmann equation in transport problems,[23] so far as I know, they have not been extensively applied to obtain approximate diagrammatic summations of the type (7). The idea is simple: The first step is to find a variational functional of $\tilde{\Lambda}$, such that variations with respect to $\tilde{\Lambda}$ yield the integral equation (7). We simplify the notation by writing (7) as

$$\sum_{\mathbf{p}'} K(\mathbf{p},\mathbf{p}')\tilde{\Lambda}(\mathbf{p}')=1\,, \tag{32}$$

where

$$K(\mathbf{p},\mathbf{p}')=\delta_{\mathbf{p},\mathbf{p}'}+\tilde{I}(\mathbf{p},\mathbf{p}')g(\mathbf{p}')\,. \tag{33}$$

We have for simplicity suppressed the parameters k and ω. The appropriate variational functional $F[\lambda(\mathbf{p})]$ is

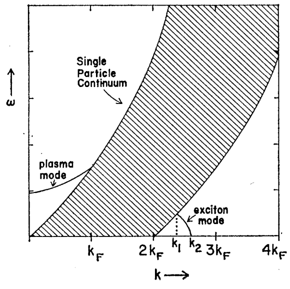

FIG. 2. A sketch of the dispersion relation of the exciton state implied by Overhauser's calculation.

$$F[\lambda]=\sum_{\mathbf{p}\mathbf{p}'} \lambda(\mathbf{p})g(\mathbf{p})K(\mathbf{p},\mathbf{p}')\lambda(\mathbf{p}')-2\sum_{\mathbf{p}} g(\mathbf{p})\lambda(\mathbf{p}) \tag{34}$$

because, clearly, the relation

$$\delta F[\lambda]/\delta\lambda(\mathbf{p})=0 \tag{35}$$

implies, since $\tilde{I}(\mathbf{p},\mathbf{p}')=\tilde{I}(\mathbf{p}',\mathbf{p})$, that

$$\sum_{\mathbf{p}'} K(\mathbf{p},\mathbf{p}')\lambda(\mathbf{p}')=1\,, \tag{36}$$

in agreement with (32). Thus the solution of (32) gives the $F(\lambda)$ an extremal value.

For certain ranges of $\mathbf{k}$ and ω, where $g_{\mathbf{k}\omega}(\mathbf{p})$ is real, we can prove that this extremal value is a minimum, provided that the particle-hole interaction $\tilde{I}$ is not too attractive. In particular, g is real for $\omega=0$ regardless of the value of $\mathbf{k}$, so that we have a minimum principle for the static dielectric constant; it is also real for $\omega<(k/m)(\frac{1}{2}k-k_{\mathrm{F}})$, which is region where Overhauser's exciton appears. In these regions, to which we restrict ourselves for the time being, the quantities g, $\tilde{\Lambda}$, and F are all real. ($\tilde{I}$ is real because of our assumption of a static particle-hole interaction.)

The proof of the minimum principle consists of three steps. First, we must define a scalar product space in which the kernel K is symmetric. Then, if $\tilde{I}$ is sufficiently weak that K is also positive definite, we can prove the minimum principle. Finally, we derive a condition on $\tilde{I}$, which, when satisfied, is sufficient to insure that K is positive definite.

We define the scalar product (A,B) between two functions $A(\mathbf{p})$ and $B(\mathbf{p})$ as

$$(A,B)=(B,A)\equiv\sum_{\mathbf{p}} g(\mathbf{p})A(\mathbf{p})B(\mathbf{p})\,. \tag{37}$$

With this definition of the scalar product, it is a matter of direct substitution of (33) to prove that K is symmetric:

$$(A,KB)=(KA,B)\,, \tag{38}$$

where we use the matrix notation

$$KA\equiv\sum_{\mathbf{p}'} K(\mathbf{p},\mathbf{p}')A(\mathbf{p}')\,,$$

and we have also used the fact $\tilde{I}(\mathbf{p},\mathbf{p}')=\tilde{I}(\mathbf{p}',\mathbf{p})$. We now

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[21] H. Mayer and B. Hietel, in *Proceedings of the International Colloquium on Optical Properties and Electronic Structure of Metals and Alloys, Paris, 1965* (North-Holland Publishing Co., Amsterdam, 1966); H. Mayer and M. H. El Naby, Z. Physik **174**, 269 (1963); **174**, 280 (1963); **174**, 289 (1963); but see also N. V. Smith, Phys. Rev. Letters **21**, 96 (1968).

[22] Recently, A. W. Overhauser [Phys. Rev. **167**, 691 (1968)] has espoused such charge fluctuations in the alkalis.

[23] E.g., see J. M. Ziman, *Electrons and Phonons* (Oxford University Press, London, 1960).

assume that $\tilde{I}$ is such that K is *positive definite*, that is,

$$(A,KA)\geq 0$$

for all A. Then we may state the *theorem:* If K is positive definite and $K\Lambda=1$, then $F[\lambda]\geq F[\Lambda]$ for all λ. The proof is simple:

$$\begin{aligned}0<((\lambda-\Lambda),\ K(\lambda-\Lambda))&\\ &=(\lambda,K\lambda)+(\Lambda,K\Lambda)-(\Lambda,K\lambda)-(\lambda,K\Lambda)\\ &=(\lambda,K\lambda)+(\Lambda,K\Lambda)-2(\lambda,1)\\ &=(\lambda,K\lambda)-2(\lambda,1)-(\Lambda,K\Lambda)+2(\Lambda,K\Lambda)\\ &=(\lambda,K\lambda)-2(\lambda,1)-(\Lambda,K\Lambda)+2(\Lambda,1).\qquad(39)\end{aligned}$$

We note that in the notation (37), the variational function (34) is

$$F[\lambda]=(\lambda,K\lambda)-2(\lambda,1),\qquad(40)$$

so that the last line of (39) implies that $F[\lambda]\geq F[\Lambda]$. Hence the function λ that minimizes F is the solution of the integral equation. Furthermore, given an approximate trial function λ depending on several parameters, the "best" values of these parameters are those that render $F(\lambda)$ a minimum. It is interesting to note that

$$-F[\Lambda]=(\epsilon-1)/2V_k,\qquad(41)$$

so that the quantity $1-2V_kF[\lambda]$ provides a lower bound for the true value of ϵ as determined by (7) and (8), for any $[\lambda]$.

Next, we derive a sufficient condition that K be positive definite, which we state in the form of a *theorem:* If $\tilde{I}$ is sufficiently weak that

$$\sum_{p'}|\tilde{I}(\mathbf{p},\mathbf{p}')|g(\mathbf{p}')<1\qquad(42a)$$

for all p, then $(A,KA)>0$ for all A, that is, K is positive definite. The proof is straightforward [note that $g(\mathbf{p})>0$]:

$$\begin{aligned}(A,KA)&=\sum_{\mathbf{p}}g(\mathbf{p})A^2(\mathbf{p})+\sum_{\mathbf{p}\mathbf{p}'}g(\mathbf{p})\tilde{I}(\mathbf{p},\mathbf{p}')g(\mathbf{p}')A(\mathbf{p})A(\mathbf{p}')\geq\sum_{\mathbf{p}}g(\mathbf{p})|A(\mathbf{p})|^2-\sum_{\mathbf{p}\mathbf{p}'}g(\mathbf{p})|\tilde{I}(\mathbf{p},\mathbf{p}')|g(\mathbf{p}')|A(\mathbf{p})||A(\mathbf{p}')|\\ &\geq\sum_{\mathbf{p}}g(\mathbf{p})|A(\mathbf{p})|^2[\sum_{\mathbf{p}'}|\tilde{I}(\mathbf{k},\mathbf{p}')|g(\mathbf{p}')]-\sum_{\mathbf{p}\mathbf{p}'}g(\mathbf{p})|\tilde{I}(\mathbf{p},\mathbf{p}')|g(\mathbf{p}')|A(\mathbf{p})||A(\mathbf{p}')|\\ &=\tfrac{1}{2}\sum_{\mathbf{p}\mathbf{p}'}g(\mathbf{p})|\tilde{I}(\mathbf{p},\mathbf{p}')|g(\mathbf{p}')[|A(\mathbf{p})|-|A(\mathbf{p}')|]^2\geq 0.\end{aligned}$$

Of course, if $\tilde{I}$ is attractive ($\tilde{I}<0$) for all **p** and **p**′, the absolute value signs are unnecessary. We also mention that it will sometimes be sufficient to replace (42a) by the weaker condition

$$[\sum_{p}g(\mathbf{p})]\max|\tilde{I}(\mathbf{p},\mathbf{p}')|<1.\qquad(42b)$$

To get a feeling for the numbers involved, we briefly discuss (42b). For $\omega=0$, $\sum_{\mathbf{p}}g(\mathbf{p})$ has its maximum value of $N(0)$ as $k\rightarrow 0$, so that the kernal is positive definite at small k if $|\tilde{I}|N(0)<1$, where $N(0)$ is the single-spin density of states at the Fermi level, $N(0)=\sum_{\mathbf{p}}\delta(\epsilon_{\mathbf{p}}-\epsilon_{\mathrm{F}})$. This means that if $\tilde{I}$ is a screened Coulomb interaction of the form (6), then the kernel K is positive definite if the screening parameter $K_s{}^2$ is at least half as big as the Fermi-Thomas screening parameter $k_{\mathrm{FT}}{}^2=8\pi e^2N(0)$. The positive definiteness of K is related to the exciton instability, in that the exciton pole cannot occur so long as K is positive definite. In fact, the conditions (42) have previously been used in this latter context.[24] In the region $k>2k_{\mathrm{F}}$, where this pole might appear, $\sum_{\mathbf{p}}g(\mathbf{p})<\frac{1}{2}N(0)$; therefore, according to (42b), the exciton pole cannot appear unless the screening of the electron-hole interaction is at least four times less effective than ordinary Fermi-Thomas screening ($K_s{}^2<\frac{1}{4}k_{\mathrm{FT}}{}^2$). The condition (42a) has been evaluated numerically for a screened Coulomb interaction in Ref. (24). The results indicate that (42a) is considerably more stringent than (42b) at high electronic densities, but comparable at lower densities.

We now use the variational principle to "solve" Eq. (7). An appropriate trial function is suggested by the calculations of Hubbard, Kleinman, and Overhauser, who all assume (by modifying the kernel) that $\tilde{\Lambda}$ is independent of **p**. On the other hand the "best" approximation of this type may be obtained by substituting a constant $\tilde{\Lambda}$ into (35), from which we obtain

$$\tilde{\Lambda}_{\mathbf{k}\omega}=\sum_{p}g_{\mathbf{k}\omega}(\mathbf{p})\Big/\Big[\sum_{\mathbf{p}}g_{\mathbf{k}\omega}(\mathbf{p})+\sum_{\mathbf{p}\mathbf{p}'}g_{\mathbf{k}\omega}(\mathbf{p})\tilde{I}(\mathbf{p},\mathbf{p}')g_{\mathbf{k}\omega}(\mathbf{p}')\Big].\qquad(43)$$

We presently will compare (43) with the calculations of the three other authors, but first we show that it is exact in several limits.

Let me make it clear that in what follows, I use the work "exact" only to denote exact solutions of (7) and (8). Thus we will be testing the validity of the approximate solutions to (7) and (8), and not the validity of (7) and (8) themselves. In particular, the fact that the relevance of (7) and (8) in the small k limit is unclear, does not eliminate the small k region as proving ground for the variational principle.

First, we consider the limit $\omega=0$, $k\rightarrow 0$. Evaluation of (43) is trivial since $g_{\mathbf{k}\omega}(\mathbf{p})\rightarrow\delta(\epsilon_{\mathbf{p}}-\epsilon_{\mathrm{F}})$. We find that

$$\tilde{\Lambda}(\mathbf{p})\rightarrow[1+\sum_{\mathbf{p}'}\tilde{I}(p_{\mathrm{F}},\mathbf{p}')\delta(\epsilon_{p'}-\epsilon_{\mathrm{F}})]^{-1}.\qquad(44)$$

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[24] P. A. Fedders and P. C. Martin, Phys. Rev. **143**, 245 (1966).

On the other hand, the exact solution of (7) in this limit is

$$\tilde{\Lambda}(\mathbf{p}) \to \Big(\{1+\sum_{\mathbf{p}'} [\tilde{I}(p_{\mathrm{F}},\mathbf{p}')-\tilde{I}(\mathbf{p},\mathbf{p}')]\delta(\epsilon_{\mathbf{p}'}-\epsilon_{\mathrm{F}})\}/ \\ [1+\sum_{\mathbf{p}'}\tilde{I}(p_{\mathrm{F}},\mathbf{p}')\delta(\epsilon_{\mathbf{p}'}-\epsilon_{\mathrm{F}})]\Big). \quad (45)$$

Hence (44) is exact for $p=p_{\mathrm{F}}$. Furthermore, substitution of either (44) or (45) into (8) gives

$$\epsilon(\mathbf{k},0)=1+\{2V_k N(0)/[1+\sum_{\mathbf{p}'}\tilde{I}(p_{\mathrm{F}},\mathbf{p}')\delta(\epsilon_{\mathbf{p}'}-\epsilon_{\mathrm{F}})]\}, \quad (46)$$

so that our variational trial function gives a dielectric constant which is exact in this limit.

Now consider the large-k limit. Since the first term in the denominator of (43) varies as k^{-2} and the second term as k^{-4}, we may write (43) as

$$\tilde{\Lambda}_{\mathbf{k}\omega} \xrightarrow[k \text{ large}]{} 1-\sum_{\mathbf{p}\mathbf{p}'} g_{\mathbf{k}\omega}(\mathbf{p})\tilde{I}(\mathbf{p},\mathbf{p}')g_{\mathbf{k}\omega}(\mathbf{p}')/ \\ \sum_{\mathbf{p}} g_{\mathbf{k}\omega}(\mathbf{p})+\cdots. \quad (47)$$

On the other hand, the exact solution of (7) yields

$$\tilde{\Lambda}_{\mathbf{k}\omega} \xrightarrow[k \text{ large}]{} 1-\sum_{\mathbf{p}'} \tilde{I}(\mathbf{p},\mathbf{p}')g_{\mathbf{k}\omega}(\mathbf{p}')+\cdots. \quad (48)$$

Thus the k dependence of (47) is correct, although the coefficient of the k^{-2} term is independent of p (by assumption) in contrast with the exact result. However, if we use (8) to calculate ϵ, then the result is the same regardless of whether we use (47) or (48):

$$\epsilon(\mathbf{k},\omega) \xrightarrow[k \text{ large}]{} 1+2V_{\mathbf{k}}[\sum_{\mathbf{p}} g_{\mathbf{k}\omega}(\mathbf{p}) \\ -\sum_{\mathbf{p}\mathbf{p}'} g_{\mathbf{k}\omega}(\mathbf{p})I(\mathbf{p},\mathbf{p}')g_{\mathbf{k}\omega}(\mathbf{p}')+\cdots], \quad (49)$$

so that the variational solution gives an exact result in this limit as well. Note that the variational calculation is exact in this limit because it reproduces the first two terms of the exact perturbation expansion of $\tilde{\Lambda}$ in powers of $\tilde{I}$; similarly, other limits that derive from this property (e.g., $k\to 0$, ω finite) will hold exactly.

It might be useful at this point to compare the variational solution (43) with the first terms in the Fredholm expansion of the solution of (7), a method applied to this problem by Hamman and Overhauser.[25] The Fredholm solution to (7) is

$$\tilde{\Lambda}=(1+\cdots)/(1+\sum_{p}\tilde{I}(p,p)g(p)+\cdots).$$

Since $\tilde{I}(p,p)=\max|\tilde{I}(p,p')|$, the first Fredholm approximant above predicts according to (42b) that the exciton instability occurs first for a screening parameter K_s^2 larger than that for which the instability occurs in the exact solution. On the other hand, the variational solution, being derived from a minimum principle, predicts that the instability occurs for a screening parameter smaller than that for which the instability occurs in the exact solution.

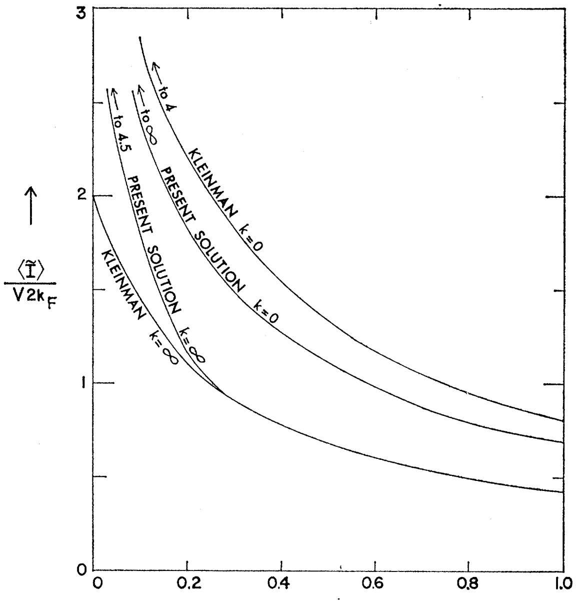

FIG. 3. Comparison of Kleinman's solution of Eqs. (6), (7), (10) for $\langle\tilde{I}\rangle$ with the present solution in the $k\to 0$ and $k\to\infty$ limits as a function of the screening parameter $\alpha=K_s^2/(2k_{\mathrm{F}})^2$. The present solution gives an ϵ according to (8) which is exact in these limits. Hubbard's solution agrees with Kleinman's in the $k=0$ limit, but gives $\langle\tilde{I}\rangle=0$ in the $k=\infty$ limit. Overhauser's solution gives $-\langle I\rangle/V_{2k_{\mathrm{F}}}=9$ in the $k=\infty$ limit.

Now we compare our calculation with that of Kleinman. To do so, we force our expression (43) into the form (10′):

$$\tilde{\Lambda}_{\mathbf{k}\omega}=[1+\langle\tilde{I}\rangle_{\mathbf{k}\omega}\Pi^{(0)}(\mathbf{k},\omega)]^{-1}, \quad (10')$$

where now $\langle\tilde{I}\rangle_{\mathbf{k}\omega}$ is a complex, frequency- and wave-vector-dependent function

$$\langle\tilde{I}\rangle_{\mathbf{k}\omega}=\sum_{\mathbf{p}\mathbf{p}'} g_{\mathbf{k}\omega}(\mathbf{p})\tilde{I}(\mathbf{p},\mathbf{p}')g_{\mathbf{k}\omega}(\mathbf{p}')/\sum_{\mathbf{p}\mathbf{p}'} g_{\mathbf{k}\omega}(\mathbf{p})g_{\mathbf{k}\omega}(\mathbf{p}'). \quad (50)$$

We now let $\tilde{I}(\mathbf{p},\mathbf{p}')$ be given by (6), and let $\omega\to 0$, and compare (50) with Kleinman's value

$$\langle\tilde{I}\rangle_k=-\left(\frac{2\pi e^2}{k^2+k_{\mathrm{F}}^2+k_s^2}+\frac{2\pi e^2}{k_{\mathrm{F}}^2+k_s^2}\right). \quad (51)$$

Because of the uncertainties in $\tilde{I}(\mathbf{p},\mathbf{p}')$, a complete numerical evaluation of (50) is probably not warranted, and we restrict our comparison to small k and large k. For large k, Eq. (50) becomes [in units of $V_{2k_{\mathrm{F}}}=4\pi e^2/(2k_{\mathrm{F}})^2$]

$$-\langle\tilde{I}\rangle/V_{2k_{\mathrm{F}}}=12[\tfrac{3}{8}-\tfrac{1}{4}\alpha-\alpha^{1/2}\tan^{-1}\alpha^{-1/2} \\ +\tfrac{1}{4}\alpha(3+\alpha)\ln(\alpha+1)/\alpha], \quad (52)$$

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[25] D. Hamman and A. W. Overhauser, Phys. Rev. **143**, 183 (1966).

where $\alpha = K_s^2/(2k_F)^2$. In the same limit (51) becomes

$$-\langle\tilde{I}\rangle/V_{2k_F} = 2(1+4\alpha)^{-1}. \quad (53)$$

Although (52) looks completely different from (53), the latter provides good approximation for reasonable values of α, as illustrated in Fig. 3. Note that if $K_s \sim k_{FT}$, then $\frac{1}{3} \lesssim \alpha \lesssim 1$ for metallic densities. The fact that (53) is very poor for small α is probably irrelevant, since one does not expect such ineffective screening. We emphasize again that in this limit the Hubbard approximation (11) is incorrect, since it predicts $\langle\tilde{I}\rangle \to 0$.

Consider now the small-k limit. Equation (50) becomes

$$\langle\tilde{I}\rangle = \ln(1+\alpha)/\alpha, \quad (54)$$

while (51) becomes

$$\langle\tilde{I}\rangle = 4(1+4\alpha)^{-1}. \quad (55)$$

As illustrated in Fig. 2, the Kleinman approximation (55) is not so good here, but on the other hand it never differs from (54) by more than $\sim 30\%$ for reasonable values of α.

At this point, we briefly mention a recent approximation for ϵ due to Singwi *et al.*[26] Here the expression for ϵ naturally falls into the form (12a) with

$$\langle\tilde{I}\rangle_k = -\frac{4\pi e^2}{Nk^2} \sum_q \frac{\mathbf{k}\cdot(\mathbf{q}+\mathbf{k})}{(\mathbf{q}+\mathbf{k})^2} [S(q)-1],$$

where $S(q)$ is the structure factor (Fourier transform of the pair function) which must be determined self-consistently. The only point we wish to make here is that at large k, this evaluation of $\langle\tilde{I}\rangle$ has the same k dependence as the original Hubbard approximation, that is $\langle\tilde{I}\rangle_k \to 0$.

We now compare with Overhauser's calculation, returning to the large-k case, the only one considered by him. Overhauser argues that additional correlation effects nullify the screening effect, so that effectively K_s^2 is very small and may be taken to be zero. Setting $\alpha = 0$ in (52) gives $-\langle\tilde{I}\rangle/V_{2k_F} = 4.5$, while on the other hand Overhauser obtains $-\langle\tilde{I}\rangle/V_{2k_F} = 9$. The factor of two difference has nothing to do with spin, and arises because phase-space considerations cause roughly half of the particle-hole interaction to become ineffective at large k. Thus, even if Overhauser's conjecture about the size of K_s is correct, he has overestimated the magnitude of $\langle\tilde{I}\rangle$. (Note that for smaller k, the discrepancy between the two figures would not be so great.)

Actually it would seem that K_s^2 is closer to k_{FT}^2 than it is to zero. Two countervailing effects are involved: first, the electrons and holes in the screening cloud correlate with each other, thus making the cloud tighter than its mean field value, whence increasing K_s^2; second, the scattered electron or hole can exchange and correlate with the electrons and holes in the screening cloud, which tends to increase the amount of scattering, and hence to decrease the effective value of K_s^2. Of course, to calculate accurately the particle-hole interaction at metallic densities is beyond the present state of the art, but to the extent that the two effects above cancel each other, the above estimate may not be unreasonable (for large k). It should also be noted that if $K_s^2 \sim k_{FT}^2$, then $\langle\tilde{I}\rangle$ is not very sensitive to the value of K_s^2; Fig. 3 shows that for $0.3 < \alpha < 1$, $\langle\tilde{I}\rangle$ only varies by a factor of 2; it is only for very small α that $\langle\tilde{I}\rangle$ shoots up to the large values used by Overhauser. In what follows, we proceed under the assumption that the best value of K_s^2 is not small, but of the order of k_{FT}^2.

We have discussed on a unified basis the approximations of Hubbard, Kleinman, and Overhauser. In all of these, $\tilde{\Lambda}$ is given by (10′), although $\langle\tilde{I}\rangle$ varies considerably. On the other hand we have shown that the best variational approximation of this type is also given by (10′), with $\langle\tilde{I}\rangle$ given by (50). The latter expression for $\langle\tilde{I}\rangle$, however, is rather unweildly; it would be desirable to have a simple numerical approximation to it. Here we are guided by the fact that we have shown by explicit calculation that the Hubbard-Kleinman method of approximating $(\mathbf{p}-\mathbf{p}')^{-2}$ in $\tilde{I}$ works very well for large k. Explicitly, the numerator of (50) is

$$\begin{aligned} -\sum_{\mathbf{p}\mathbf{p}'} &(\omega+i\eta+\epsilon_{\mathbf{p}}-\epsilon_{\mathbf{p}+\mathbf{k}})^{-1}(\omega+i\eta+\epsilon_{\mathbf{p}'}-\epsilon_{\mathbf{p}+\mathbf{k}})^{-1} \\ &\times\Bigg\{ f_{\mathbf{p}+\mathbf{k}}(1-f_{\mathbf{p}})\frac{4\pi e^2}{(\mathbf{p}-\mathbf{p}')^2+K_s^2} f_{\mathbf{p}'+\mathbf{k}}(1-f_{\mathbf{p}'}) \\ &+f_{\mathbf{p}}(1-f_{\mathbf{p}+\mathbf{k}})\frac{4\pi e^2}{(\mathbf{p}-\mathbf{p}')^2+K_s^2} f_{\mathbf{p}'}(1-f_{\mathbf{p}'+\mathbf{k}}) \\ &-f_{\mathbf{p}}(1-f_{\mathbf{p}+\mathbf{k}})\frac{4\pi e^2}{(\mathbf{p}-\mathbf{p}')^2+K_s^2} f_{\mathbf{p}'+\mathbf{k}}(1-f_{\mathbf{p}'}) \\ &-f_{\mathbf{p}+\mathbf{k}}(1-f_{\mathbf{p}})\frac{4\pi e^2}{(\mathbf{p}-\mathbf{p}')^2+K_s^2} f_{\mathbf{p}'}(1-f_{\mathbf{p}'+\mathbf{k}})\Bigg\}. \end{aligned} \quad (56)$$

In approximating (56) we must be careful not to destroy the exact invariance (16). We must also be careful not to introduce any spurious imaginary parts. For this reason we have added and subtracted the factors $f_{\mathbf{p}+\mathbf{k}}f_{\mathbf{p}}$ and $f_{\mathbf{p}'+\mathbf{k}}f_{\mathbf{p}'}$ in writing (56). In the first two terms in the curly brackets we replace $4\pi e^2[(\mathbf{p}-\mathbf{p}')^2+K_s^2]^{-1}$ by $4\pi e^2[k_F^2+K_s^3]^{-1}$. These two terms give the dominant contribution for large k and this approximation to them has been explicitly tested in Sec. III. On the other hand, in the last two terms in the curly brackets, we replace $4\pi e^2[(\mathbf{p}-\mathbf{p}')^2+K_s^2]^{-1}$ by $4\pi e^2[k^2+k_F^2+K_s^2]^{-1}$, because at large k the Fermi factors associated with this term force it to be small. We thus

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[26] K. S. Singwi, M. P. Tosi, and A. Sjölander, Nuovo Cimento **54**, B160 (1968); J. Hubbard, Phys. Letters **25A**, 709 (1967); K. S. Singwi, M. P. Tosi, and R. H. Land, Phys. Rev. (to be published).

obtain

$$\langle\tilde{I}\rangle=\left(\frac{4\pi e^2}{k_{\mathrm{F}}^2+K_s^2}\{[\chi(\mathbf{k},\omega)]^2+[\chi^*(-\mathbf{k},\,-\omega)]^2\}\right.$$
$$\left.+\frac{4\pi e^2}{k^2+k_{\mathrm{F}}^2+K_s^2}[2\chi(\mathbf{k},\omega)\chi^*(-\mathbf{k},\,-\omega)]\right)$$
$$\times[\chi(\mathbf{k},\omega)+\chi^*(-k,\,-\omega)]^{-2},\quad(57)$$

where

$$\chi(\mathbf{k},\omega)=-\sum_{\mathbf{p}}\frac{f_{\mathbf{p}}(1-f_{\mathbf{p}+\mathbf{k}})}{\omega+i\eta+\epsilon_{\mathbf{p}}-\epsilon_{\mathbf{p}+\mathbf{k}}}.\quad(58)$$

The corresponding values of ϵ and Λ are given by Eq. (12). Equation (57) should provide a reasonable estimate of the size of the correlation and exchange contributions to Λ. For more accurate values one would have to evaluate (50) numerically. We do not think this effort would be justified in view of the uncertainty in the form of the particle-hole interaction. Note that (57) is different from Kleinman's approximation, even though both used the Hubbard method of approximating the integrals. Our relation does not violate the exact symmetry (16), and does not have spurious imaginary parts in regions of $\mathbf{k}$ and ω where the exact solution of (7) is real. We should also mention again that (57) is not valid for small k because (6) and (7) are not valid for small k.

In the limit $\omega=0$, (57) reduces exactly to Kleinman's value (51). Hence in this limit

$$\begin{aligned}\Lambda_{k,0}^{-1}&=1+[1-f(k)]F(k),\\ \epsilon(k,0)&=1+F(k)/[1-f(k)F(k)],\end{aligned}\quad(59)$$

where[26]

$$f(k)=\frac{1}{4}\left(\frac{k^2}{k^2+k_{\mathrm{F}}^2+K_s^2}+\frac{k^2}{k_{\mathrm{F}}^2+K_s^2}\right),$$

$$F(k)=\frac{k_{\mathrm{FT}}^2}{k^2}\left[\frac{1}{2}+\frac{k_{\mathrm{F}}}{2k}\left(1-\frac{k^2}{4k_{\mathrm{F}}^2}\right)\ln\left|\frac{k+2k_{\mathrm{F}}}{k-2k_{\mathrm{F}}}\right|\right].$$

The evaluation of $F(k)$ above has approximated ϵ_p by $p^2/2m$. As pointed out by Geldart and Vosko,[2] such an approximation results in the failure of the k^{-6} terms in $\epsilon(k,0)$ to cancel, even though the leading large-k dependence of $\tilde{\Lambda}$ is still correct. Numerically this is probably not important, but if it is one should evaluate $F(k)$ from (58) without replacing ϵ_p by $p^2/2m$, as discussed by Kleinman. The use of the original Hubbard approximation for ϵ would be better at large k, than the use of Kleinman's original form above with $\epsilon_p=p^2/2m$.

We remark that although (59) has no *a priori* validity for small k, the Ward identity (5) shows that our expression for ϵ is qualitatively correct in this region in that the coefficient of the k^{-2} term is considerably larger than k_{FT}^2. It is therefore tempting to pick K_s^2 such that this compressibility limit is right, and to use (59) as an interpolation formula between large and small k, following the procedure espoused by Geldart and Vosko.[2] Thus we pick K_s^2 as given by Nozières-Pines interpolation formula[9]

$$k_{\mathrm{F}}^2/(K_s^2+k_{\mathrm{F}}^2)=\tfrac{1}{2}[1+0.158(k_{\mathrm{FT}}/2k_{\mathrm{F}})^2].\quad(60)$$

For the higher-density metals (60) yields values of K_s^2 close to but somewhat less than k_{FT}^2, as anticipated from earlier arguments. Of course for small k, the values of Λ and ϵ can only be consistent to the extent that $Zm^*/m\sim 1$, which at best limits one to the high-density metals. We mention, however, that the value of $\tilde{\Lambda}$ implied by (59) is considerably less sensitive to the magnitude of k than Hubbard's $\tilde{\Lambda}$ in the range $0<k<2k_{\mathrm{F}}$, as might be expected from Rice's calculations.

We conclude this section by emphasizing that the formulas derived here should be treated with caution. For the high-density metals we feel that they are reasonable and give simple estimates of the magnitudes of the corrections to be expected. Screening calculations known *a priori* to be accurate at metallic densities do not exist, and are unlikely to exist in the near future.

V. GROUND-STATE ENERGY

We raised the question earlier of what effect the rather larger value of $\langle\tilde{I}\rangle$ will have on the standard calculations of the correlation energy of the electron gas. Here we use our variational solution for ϵ to derive an expression for the correlation energy. As usual the correlation energy is written as

$$E_{\mathrm{corr}}=\sum_k E_c(k),\quad(61)$$

with[6,7]

$$E_{\mathrm{corr}}(k)=-\int_0^{e^2}\frac{dg}{g}\int_0^{\infty}\frac{d\omega}{2\pi}$$
$$\times\operatorname{Im}\{[(\epsilon(\mathbf{k},\omega))^{-1}-1]+2V_k\Pi^{(0)}(\mathbf{k},\omega)\}.\quad(62)$$

This is the normal coupling constant integration, where all factors of e^2 contained implicitly in the curly brackets are replaced by g. According to our variational calculation

$$\frac{1}{\epsilon}-1=-\frac{2V_k\Pi^{(0)}}{1+[2V_k+\langle\tilde{I}\rangle]\Pi^{(0)}},\quad(63)$$

where $\langle\tilde{I}\rangle$, a complex function of k and ω, is given by (50). For small k, this value of $\langle\tilde{I}\rangle$ is not correct, but this is irrelevant because the terms in the square brackets in the denominator of (63) are dominated by V_k in this limit, so that the integral (62) is insensitive to the value of $\langle\tilde{I}\rangle$ in this limit.[4] Furthermore, in performing the coupling constant integration, we assume that the particle-hole interaction $\tilde{I}$ and hence $\langle\tilde{I}\rangle$ is proportional to g; this is only a good approximation for large k, but

$\langle\tilde{I}\rangle$ is important only in this regime. We obtain

$$E_{\mathrm{corr}}(k)=-\int_0^\infty\frac{d\omega}{2\pi}$$

$$\times\operatorname{Im}\left\{2V_k\Pi^{(0)}\left[1-\frac{\ln(1+[2V_k+\langle\tilde{I}\rangle]\Pi^{(0)})}{[2V_k+\langle\tilde{I}\rangle]\Pi^{(0)}}\right]\right\}. \quad (64)$$

Numerical evaluation of (64) would be difficult. Instead, we discuss its limiting forms for small and large k. For small k, $\langle\tilde{I}\rangle$ may be neglected and (64) reduces to the random phase approximation, which is known to be accurate in this limit.[6] On the other hand, for large k we may expand the logarithm to obtain

$$E_{\mathrm{corr}}(k)\simeq-\int_0^\infty\frac{d\omega}{2\pi}\operatorname{Im}\{V_k(\Pi^{(0)})^2[2V_k+\langle\tilde{I}\rangle]\}. \quad (65)$$

For convenience define

$$E_{\mathrm{corr}}(k)=E_d(k)+E_e(k), \quad (66)$$

with

$$E_d(k)=-\int_0^\infty\frac{d\omega}{2\pi}\operatorname{Im}2V_k^2(\Pi^{(0)})^2, \quad (67\mathrm{a})$$

$$E_e(k)=-\int_0^\infty\frac{d\omega}{2\pi}\operatorname{Im}V_k\langle\tilde{I}\rangle(\Pi^{(0)})^2. \quad (67\mathrm{b})$$

Equation (67a) is easily evaluated, yielding

$$E_d(k)=-2V_k^2\sum_{\mathrm{pp'}}\frac{f_{\mathrm{p}}(1-f_{\mathrm{p+k}})f_{\mathrm{p'}}(1-f_{\mathrm{p'+k}})}{\epsilon_{\mathrm{p+k}}+\epsilon_{\mathrm{p'+k}}-\epsilon_{\mathrm{p}}-\epsilon_{\mathrm{p'}}}. \quad (68)$$

Notice that $E_d(k)$ is just the direct Coulomb integral of second-order perturbation theory. To evaluate (67b), we use the expression (50) for $\langle\tilde{I}\rangle$, obtaining

$$\begin{aligned}\langle\tilde{I}\rangle\Pi_0^2=\sum_{\mathrm{pp'}}\Bigg\{&\frac{f_{\mathrm{p+k}}(1-f_{\mathrm{p}})\tilde{I}(\mathbf{p},\mathbf{p}')f_{\mathrm{p'+k}}(1-f_{\mathrm{p'}})}{(\omega+i\eta+\epsilon_{\mathrm{p}}-\epsilon_{\mathrm{p+k}})(\omega+i\eta+\epsilon_{\mathrm{p'}}-\epsilon_{\mathrm{p'+k}})}\\&+\frac{f_{\mathrm{p}}(1-f_{\mathrm{p+k}})\tilde{I}(\mathbf{p},\mathbf{p}')f_{\mathrm{p'}}(1-f_{\mathrm{p'+k}})}{(\omega+i\eta+\epsilon_{\mathrm{p}}-\epsilon_{\mathrm{p+k}})(\omega+i\eta+\epsilon_{\mathrm{p'}}-\epsilon_{\mathrm{p'+k}})}\\&-\frac{f_{\mathrm{p}}(1-f_{\mathrm{p+k}})\tilde{I}(\mathbf{p},\mathbf{p}')f_{\mathrm{p'+k}}(1-f_{\mathrm{p'}})}{(\omega+i\eta+\epsilon_{\mathrm{p}}-\epsilon_{\mathrm{p+k}})(\omega+i\eta+\epsilon_{\mathrm{p'}}-\epsilon_{\mathrm{p'+k}})}\\&-\frac{f_{\mathrm{p+k}}(1-f_{\mathrm{p}})\tilde{I}(\mathbf{p},\mathbf{p}')f_{\mathrm{p'}}(1-f_{\mathrm{p'+k}})}{(\omega+i\eta+\epsilon_{\mathrm{p}}-\epsilon_{\mathrm{p+k}})(\omega+i\eta+\epsilon_{\mathrm{p'}}-\epsilon_{\mathrm{p'+k}})}\Bigg\}. \quad (69)\end{aligned}$$

Notice that it is the first two terms in the curly brackets in (69) which give the predominant contribution to $\langle\tilde{I}\rangle$ in the static limit, and are the ones that cause our approximation to have a larger value of $\langle\tilde{I}\rangle$ than the Hubbard approximation—these are the terms that have the different k dependence. Notice on the other hand that the frequency integral of the imaginary part of these terms is identically zero. Therefore they do not contribute to $E_e(k)$ at all. In the last two terms in (69), we replace $\tilde{I}(\mathbf{p},\mathbf{p}')$ by the Coulomb interaction $-V_{\mathrm{p-p'}}$, because the Fermi functions there force $|\mathbf{p}-\mathbf{p}'|$ to be large when k is large. Hence we find that

$$E_e(k)=V_k\sum_{\mathrm{pp'}}V_{\mathrm{p+p'+k}}\frac{f_{\mathrm{p}}(1-f_{\mathrm{p+k}})f_{\mathrm{p'}}(1-f_{\mathrm{p'+k}})}{\epsilon_{\mathrm{p+k}}+\epsilon_{\mathrm{p'+k}}-\epsilon_{\mathrm{p}}-\epsilon_{\mathrm{p'}}}. \quad (70)$$

Notice that $E_e(k)$ as given by (70) is just the exchange integral of second-order perturbation theory.

Thus the interpolation scheme for evaluating the integral (61) which follows naturally from the approximation (50) is identical to the Nozières-Pines scheme.[6] Actually, for computational reasons Nozières and Pines replace $E_e(k)$ by $-\frac{1}{2}E_d(k)$, which is only exact at infinite k, although a good approximation for smaller k. Here the exact form comes out of the coupling-constant integration automatically.

We might also mention that if we had used the approximation (57) for $\langle\tilde{I}\rangle$ rather than the more exact form (50), we would have found that for large k

$$E_{\mathrm{corr}}(k)=\{1-\tfrac{1}{2}[k^2/(k^2+k_{\mathrm{F}}^2+K_s^2)]\}E_d(k) \quad (71)$$

with $E_d(k)$ given by (67). This is precisely the form of $E_{\mathrm{corr}}(k)$ in the Hubbard approximation for large k.

VI. CONCLUSIONS

We have touched on two questions here, first of solving the integral equation for the vertex function for large k, and second of determining the form of the particle-hole interaction itself. We believe that the variational principle provides a reasonable answer to the first. We have, however, said little about the second more difficult and more important question. Indeed, we have shown that the momentum transfer $|\mathbf{p}-\mathbf{p}'|$ across the part of the particle-hole interaction does not increase indefinitely with k, but remains $\sim k_{\mathrm{F}}$. This means that frequency-dependent screening and vertex corrections to the particle-hole interaction itself are bound to have some importance even at large k. These have not been considered, except to the extent that they can be lumped into one screening parameter. Ideally one should put the process through another iteration, using our vertex and dielectric functions to calculate the full frequency and wave-vector-dependent particle-hole interaction, then resolve the integral equation to check for self-consistency.

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