Fig. 1 are incorrect. The correct expressions are $\psi_3=\psi_{3/2}-e^{i\phi}\epsilon\psi_{1/2}$ and $\psi_4=\psi_{-3/2}-e^{-i\phi}\epsilon\psi_{-1/2}$. S. L. Segel and R. G. Barnes [Phys. Rev. Letters **15**, 886 (1965)] have observed the $\nu_{12}=2\nu_M$ transition for $\theta=90°$ in several polycrystalline samples including sodium bromate. It should be possible to enhance or invert this signal by pumping, although special attention must be given to the direction of the pump H_1 for $\theta=90°$ to ensure nonzero induced transition probabilities. However, we do not expect to obtain W_1/W_2 by spin-pumping a polycrystalline sample because for $\theta=90°$ the P_{ij} for the pump transitions differ only by small terms proportional to ϵ.

ACKNOWLEDGMENTS

We wish to thank M. M. Hulse for electronic services and O. Roloff for machine work and assistance in the assembly of the apparatus.

PHYSICAL REVIEW VOLUME 143, NUMBER 1 MARCH 1966

Electron-Gas Spin Susceptibility*

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(Received 23 September 1965)

The wave-vector-dependent spin susceptibility of an electron gas is calculated taking dynamically screened electron interactions into account. A quasiparticle approach is developed to deal with the self-energy and screening effects of the electron correlations, and the energy and mass of a quasiparticle at the Fermi surface are calculated for a wide density range. The susceptibility is found using a linearized self-consistent-field treatment of the quasiparticles and numerical solution of the resulting integral equation. It does not show singular or anomalous behavior at large wave vector as in the Hartree-Fock approximation. The density dependence of the zero-wave-vector susceptibility is found to be in better agreement with experiment than that of previous calculations. Statically screened interactions are also used in a series of calculations, and it is shown that a long- but finite-range interaction can lead to anomalies in the susceptibility at large wave vectors.

1. INTRODUCTION

THE effect of the Coulomb interaction on the magnetic properties of the electrons in a simple metallic conduction band has received a good deal of attention recently. One of the authors has shown that it renders the paramagnetic plane-wave state of the free-electron-gas model unstable within the Hartree-Fock (HF) approximation, an antiferromagnetic spin-density wave (SDW) state having lower energy.[1] The long-range components of the Coulomb interaction are most important in creating this instability. Correlation corrections to the HF approximation for the paramagnetic electron gas have been studied extensively, and it is agreed that the long-range components of the Coulomb interaction make a major contribution to the correlation energy, especially at high densities.[2] Therefore it is apparent that correlation corrections should be applied to a calculation of the SDW instability. The evaluation of the energy of a SDW state with correlation is an extremely difficult undertaking, however, and our goal in this paper is more modest. By calculating the wave-vector-dependent spin susceptibility of the paramagnetic state and including correlations, the stability of this state under infinitesimal deformations can be investigated, and this is the calculation we shall discuss.

The wave-vector-dependent spin susceptibility is defined by the following thought experiment: A static magnetic field $\mathbf{H}(\mathbf{x})=H_0\boldsymbol{\varepsilon}\cos(\mathbf{Q}\cdot\mathbf{x})$ is applied to the electrons, and the spin magnetization is measured. For the free-electron gas and for small H_0, it has the same spatial dependence and polarization, $\mathbf{M}(\mathbf{x})=M_0\boldsymbol{\varepsilon}\cos(\mathbf{Q}\cdot\mathbf{x})$. The susceptibility is defined as $\chi(Q)=M_0/H_0$ in the limit as H_0 goes to zero. In the approximation we shall consider, neglecting field-orbit spin-orbit, and dipolar spin-spin couplings, χ does not depend on the angle between $\boldsymbol{\varepsilon}$ and $\mathbf{Q}$. The change in internal energy associated with the magnetization is proportional to $M_0^2/\chi(Q)$. Therefore, if the paramagnetic state is unstable, we should expect to calculate a nega-

* The portion of this research, which was performed at the Massachusetts Institute of Technology, was supported by the Office of Naval Research, Contract No. Nonr-1841(72).

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[1] A. W. Overhauser, Phys. Rev. **128**, 1437 (1962).

[2] For a review of much of this work, see D. Pines, *The Many Body Problem* (W. A. Benjamin, Inc., New York, 1961).

tive χ for certain Q values, and for the negative regions to be separated from the positive regions (corresponding to deformations which increase the energy) by singularities. Of course such a result would not be physical, since the stable ground state must be used as the starting point for a meaningful calculation of χ, but it would yield important information about the paramagnetic state.

In the event that the correlations do stabilize the paramagnetic state relative to small deformations, a significant interaction effect upon χ might remain. This could modify the strength and spatial dependence of indirect exchange interactions between localized magnetic moments in metals. The widely known theoretical treatments of indirect exchange by Ruderman and Kittel[3] and others[4,5] neglect electron interactions. Recent measurements of the spatial dependence of the s-band polarization near nonmagnetic impurities in iron do not agree with the Ruderman-Kittel result.[6] These measurements might be interpreted by assuming that $\chi(Q)$ is strongly peaked near $Q=2k_F$ (where k_F is the Fermi momentum) as a result of the electron interactions,[7] a reasonable form to consider since χ has singularities near $Q=2k_F$ in the HF approximation.[1] It has also been suggested that these measurements can be explained by using more realistic electronic wave functions in computing the s-d interaction and neglecting s-band electron interactions.[8] The present calculation should aid in resolving this point.

The effect of interactions on $\chi(Q)$ was previously treated by Wolff in an approximation equivalent to linearized HF theory.[9] He solved the pertinent integral equation for a fermion gas with delta-function interactions, and found that no SDW instability occurred in this system. We shall rederive Wolff's results in Sec. 2 by an alternative method which will permit us to give a physical interpretation to the unknown function appearing in his integral equation. Several workers have investigated the stability of the paramagnetic state in this approximation without introducing $\chi(Q)$,[10–12] and have obtained results similar to those discussed.

The uniform susceptibility, $\chi(0)$, is amenable to calculation using the techniques developed for the electron gas correlation energy, and several calculations of this sort have been carried out.[13–15] $\chi(0)$ is also more accessible experimentally, since the Knight shift[16] provides a measure of it. The zero-wave-vector limit of the present results will be compared with the other calculations and with experimental results for the alkali metals.

Correlation effects were incorporated in the $\chi(Q)$ calculation using a quasiparticle approach and Sec. 3 is devoted to this development. In Sec. 4, the method of solution of the integral equation giving $\chi(Q)$ is discussed. Before calculating $\chi(Q)$ using realistic correlation corrections, a series of calculations based on Wolff's approximation[9] and using a statically screened interaction were performed, and their results are given in Sec. 5. The results of the realistic calculation are given in Sec. 6.

2. HARTREE-FOCK THEORY OF THE SUSCEPTIBILITY

In this section, Wolff's theory of the susceptibility[9] will be rederived using standard HF theory[17] rather than equation-of-motion or field-theoretic methods. The fermion system we shall consider has the Hamiltonian

$$H=\sum_i p_i^2/2m+\sum_{i<j} V(\mathbf{x}_i-\mathbf{x}_j). \tag{1}$$

If a perturbing magnetic field of the form discussed in Sec. 1 is introduced, with the polarization vector taken in the z direction, the perturbing Hamiltonian representing the Zeemann interaction is

$$H'=-\mu_B H_0 \sum_i (S_z)_i \cos\mathbf{Q}\cdot\mathbf{x}_i, \tag{2}$$

where μ_B is the Bohr magneton, and H_0 is the amplitude of the applied magnetic field. The matrix elements of (2) between single-particle plane-wave states are

$$\langle \mathbf{k}'\sigma' | H' | \mathbf{k}\sigma\rangle = -\tfrac{1}{2}\mu_B H_0 (S_z)_{\sigma'\sigma}[\delta_{\mathbf{k}',\mathbf{k}+\mathbf{Q}}+\delta_{\mathbf{k}',\mathbf{k}-\mathbf{Q}}]. \tag{3}$$

In order to find the ground state of the perturbed system in the HF approximation, the simplest procedure is to guess a form for the single-particle Hamiltonian, find its eigenstates, and then examine the validity of our guess by computing the self-consistent field. It is physically reasonable to expect the self-consistent field to have a form similar to the applied perturbation. The only simple generalization of (3) is to make the amplitude of the nonzero matrix elements of the self-consistent field a function of $\mathbf{k}$ instead of a constant. Based on this consideration, let us assume that the single-

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[10] K. Sawada and N. Fukuda, Progr. Theoret. Phys. (Kyoto) **25**, 653 (1960).
[11] A. Yoshimori, Phys. Rev. **124**, 326 (1961).
[12] F. Iwamoto and K. Sawada, Phys. Rev. **126**, 887 (1961); N. Fukada, F. Iwamoto, and K. Sawada, *ibid.* **135**, A932 (1964), Appendix A.
[13] D. Pines, in *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic Press Inc., New York, 1955), Vol. 1, p. 367.
[14] M. Shimizu, J. Phys. Soc. Japan **15**, 376 (1960).
[15] S. Silverstein, Phys. Rev. **130**, 1703 (1963).
[16] W. D. Knight, Phys. Rev. **76**, 1259 (1949).
[17] See, for example, A. Messiah, *Quantum Mechanics*, translated by J. Potter (North-Holland Publishing Company, Amsterdam, 1962), Vol. 2, pp. 773–81.

particle HF Hamiltonian has the form

$$\langle \mathbf{k}'\sigma'|H_{\mathrm{HF}}|\mathbf{k}\sigma\rangle = E_{\mathbf{k}}\delta_{\mathbf{k}',\mathbf{k}}\delta_{\sigma',\sigma} + \tfrac{1}{2}(S_z)_{\sigma'\sigma} \times [U(\mathbf{k}+\mathbf{Q}/2)\delta_{\mathbf{k}',\mathbf{k}+\mathbf{Q}} + U(\mathbf{k}-\mathbf{Q}/2)\delta_{\mathbf{k}',\mathbf{k}-\mathbf{Q}}], \quad (4)$$

where we have attempted to represent the total effective field by a single real function U, whose arguments have been written in the indicated manner to make H_{HF} Hermitian.

Since the susceptibility is defined as the linear response, it is only necessary to consider the limit of small applied fields. As long as the paramagnetic plane-wave state is stable, the off-diagonal portion of the self-consistent field must go to zero as the applied field goes to zero, and such stability is a basic assumption of this calculation. Therefore it is valid to find the perturbed single-particle states (which go over into plane-wave states as H_0 goes to zero) to first order in perturbation theory. If $\varphi_{\mathbf{k},\sigma}$ and $\psi_{\mathbf{k},\sigma}$ denote the unperturbed and perturbed wavefunctions, we find

$$\psi_{\mathbf{k},\sigma} = \varphi_{\mathbf{k},\sigma} - \frac{\tfrac{1}{2}(S_z)_{\sigma\sigma}U(\mathbf{k}+\mathbf{Q}/2)}{E_{\mathbf{k}+\mathbf{Q}}-E_{\mathbf{k}}}\varphi_{\mathbf{k}+\mathbf{Q},\sigma} - \frac{\tfrac{1}{2}(S_z)_{\sigma\sigma}U(\mathbf{k}-\mathbf{Q}/2)}{E_{\mathbf{k}-\mathbf{Q}}-E_{\mathbf{k}}}\varphi_{\mathbf{k}-\mathbf{Q},\sigma}. \quad (5)$$

Since the single-particle energies are unchanged to first order in U, except for a negligible number ($\propto U^2$) of states near the energy gaps associated with the vanishing of energy denominators in (5), the perturbed state may be taken to be simply a filled Fermi sphere of $\psi_{\mathbf{k},\sigma}$.

The plane wave matrix elements of the interaction contribution to H_{HF} are given by

$$\langle \mathbf{k}'\sigma'|V|\mathbf{k}\sigma\rangle = \sum_{\mathbf{k}''<k_F;\sigma''s_1s_2}\int d^3x_1 d^3x_2 \{\varphi_{\mathbf{k}'\sigma'}^*(\mathbf{x}_1s_1)\varphi_{\mathbf{k}\sigma}(\mathbf{x}_1s_1) \times V(\mathbf{x}_1-\mathbf{x}_2)\psi_{\mathbf{k}''\sigma''}^*(\mathbf{x}_2s_2)\psi_{\mathbf{k}''\sigma''}(\mathbf{x}_2s_2) - \psi_{\mathbf{k}''\sigma''}^*(\mathbf{x}_1s_1) \times \varphi_{\mathbf{k}\sigma}(\mathbf{x}_1s_1)V(\mathbf{x}_1-\mathbf{x}_2)\varphi_{\mathbf{k}'\sigma'}^*(\mathbf{x}_2s_2)\psi_{\mathbf{k}''\sigma''}(\mathbf{x}_2s_2)\}. \quad (6)$$

In substituting the wave functions (5) in (6), terms of second order in U must be neglected to be consistent with the linearization previously imposed on the wave functions. When the spin sums in (6) are carried out, it is found that the direct term makes no contribution, since there is no density perturbation to first order. The exchange term has both diagonal and off-diagonal elements, and it is found that the guessed form (4) is correct if we make the identifications

$$E_{\mathbf{k}} = k^2/2m - \sum_{\mathbf{k}'} v(\mathbf{k}-\mathbf{k}')n_{\mathbf{k}'}, \quad (7)$$

(we take $\hbar=1$), and

$$U(\mathbf{k}) = -\mu_B H_0 + \sum_{\mathbf{k}'} \frac{n_{\mathbf{k}'-\mathbf{Q}/2}-n_{\mathbf{k}'+\mathbf{Q}/2}}{E_{\mathbf{k}'+\mathbf{Q}/2}-E_{\mathbf{k}'-\mathbf{Q}/2}} v(\mathbf{k}-\mathbf{k}')U(\mathbf{k}'), \quad (8)$$

where $v(q)$ is the Fourier transform of $V(x)$, and $n_{\mathbf{k}}$ is the occupation number,

$$n_{\mathbf{k}} = \begin{cases} 1, & k<k_F \\ 0, & k>k_F. \end{cases} \quad (9)$$

Expression (7) is the usual HF single-particle energy. Equation (8) can be considered simply as a statement that the self-consistent field is equal to the sum of the applied and average exchange contributions. It forms an integral equation determining U. The integral in (8) is well defined, since the volume factor in the numerator vanishes when the energy denominator vanishes in such a manner that the ratio approaches a finite limit [for a nonsingular $v(q)$].

The spin density in the ground state of the perturbed system is given by

$$\langle S_z(\mathbf{x})\rangle = \sum_{k<k_F;\sigma\sigma'} \psi_{\mathbf{k},\sigma'}^*(S_z)_{\sigma'\sigma}\psi_{\mathbf{k},\sigma}. \quad (10)$$

After substituting the wavefunctions (5) into (10), it is found that the magnetization does, in fact, have the same spatial variation as the applied magnetic field. To obtain the susceptibility, we note that (8) is a linear integral equation, so that U is proportional to the inhomogeneous term $-\mu_B H_0$. The magnetization is a linear functional of U, so if $\tilde{U}$ is defined as the solution to (8) with $-\mu_B H_0$ replaced by unity, χ is given by

$$\chi(Q) = 2\mu_B^2 \sum_{\mathbf{k}} \frac{n_{\mathbf{k}-\mathbf{Q}/2}-n_{\mathbf{k}+\mathbf{Q}/2}}{E_{\mathbf{k}+\mathbf{Q}/2}-E_{\mathbf{k}-\mathbf{Q}/2}}\tilde{U}(\mathbf{k}). \quad (11)$$

Equations (8) and (11) are equivalent to Wolff's (12) and (13).[9]

In the limit of vanishing interaction $\tilde{U}=1$, and (11) gives the susceptibility of a noninteracting electron gas. In the case of a repulsive interaction, the kernel in (8) will be positive, so that a positive feedback mechanism will increase the effective field each electron sees, and hence enhance the susceptibility. If the feedback is stronger than necessary to make the magnetization self-sustaining for some values of Q, a formal solution of (8) will still be obtained, but the χ computed will be negative, indicating that the deformed ground state has a lower energy, and that the assumption of the stability of the paramagnetic state was incorrect.

3. QUASIPARTICLE FORMULATION

The derivation of the last section demonstrated that calculating $\chi(Q)$ consists essentially of finding the new ground state of the electron gas in the presence of a stationary perturbation. In seeking a means of including correlation, we decided to exploit this simplifying feature of the problem, and avoid the artificial introduction of time dependence frequently made to derive a many-body perturbation expansion.[2] This can be done using an approach similar to that of Landau's Fermi-liquid

theory,[18] but distinct in several respects. Following Landau, we use a Fermi sphere of independent quasiparticles to represent a much more complicated ground state of the electrons. Landau's theory is designed to cope with dynamic situations in which real excitations occur, and since single-particle excitations far from the Fermi surface decay rapidly, the quasiparticle model of such an excited state is not a good one. For this reason his theory confines itself to low-frequency and long-wavelength external forces, which can only create excitations near the Fermi surface. In the $\chi(Q)$ calculation, however, we do not deal with excited states. The applied magnetic field causes an electron in state $\mathbf{k}$ to spend some of its time in $\mathbf{k}\pm\mathbf{Q}$, but this simply describes the modification of the ground state. The fact that an electron injected into the electron gas with $\mathbf{k}\pm\mathbf{Q}$ would lose energy rapidly if this state were far from the Fermi surface is immaterial. We shall use a quasiparticle model to treat our static problem for large Q as well as small, since only the dressing of the bare electrons, which changes their energy-momentum relation and screens their interactions, is important.

The frequently employed quasiparticle models postulating Thomas-Fermi-screened[19] or delta-function interactions were considered inadequate because of the importance of dynamic effects in electron-gas screening. Consider a classical point change moving through an electron gas with velocity $\mathbf{v}$. The potential produced by the $\mathbf{q}$ Fourier component of this charge distribution is proportional to $[\epsilon(q,\mathbf{q}\cdot\mathbf{v})]^{-1}$, where $\epsilon(q,\omega)$ is the wave vector and frequency-dependent retarded longitudinal dielectric function. If the self-consistent field approximation for $\epsilon(q,\omega)$ is used,[20] it is found that $\mathrm{Re}\epsilon(q,\omega)$ changes sign near $\omega=qv_F$, where v_F is the Fermi velocity. Thus if the classical charge is moving with v near v_F, the screened potential will be highly anisotropic, and any static approximation extremely poor. Since electrons near the Fermi surface are most important for the SDW instability in HF theory,[1] it was considered that the dynamic screening effects were likely to be of importance in the $\chi(Q)$ calculation.

The effective Hamiltonian describing the quasiparticles is derived by finding the average effect of an electron gas in its ground state on a few distinguished "test electrons." The reasonable hypothesis is then made that all the electrons can be described by this Hamiltonian, and exchange symmetry among the quasiparticles is reintroduced. The fact that we average over coordinates and then present a Hamiltonian which appears to have access to a full electron-gas Hilbert space makes this approach nonrigorous. The screening fluctuations having been taken into account should result in a restriction on the states available to the quasiparticle system, similar to the subsidiary condition in Bohm and Pines' early treatment of screening.[21] However, we shall use the effective Hamiltonian to treat a spin-density disturbance, and it is eminently reasonable that this mode of deformation would not violate the restrictions of a rigorous theory. (Using it to calculate density fluctuations, however, might be questionable.)

The formal technique used to derive the effective Hamiltonian for the test electrons in the electron-gas dielectric medium is similar to that used by Kittel for electrons in a phonon gas.[22] We write the Hamiltonian in three parts,

$$H=H_0+H_1+H_2. \tag{12}$$

The first includes the kinetic energy of the test electrons, which will be represented by their creation and destruction operators $a^\dagger$ and a, and the total Hamiltonian for the dielectric,

$$H_0=\sum_{\mathbf{k}\sigma}\epsilon_{\mathbf{k}}a_{\mathbf{k},\sigma}^\dagger a_{\mathbf{k},\sigma}+H_d, \tag{13}$$

where $\epsilon_{\mathbf{k}}=k^2/2m$. H_d will not be written out, but will be represented by its eigenstates $|n\rangle$ with eigenvalues ω_n. The energy scale will be chosen so that its ground state $|0\rangle$ has energy zero. The second term in (12) is the test electron-dielectric interaction,

$$H_1=\sum_{\mathbf{k}\mathbf{q}\sigma}v(q)\rho_{-\mathbf{q}}a_{\mathbf{k}+\mathbf{q},\sigma}^\dagger a_{\mathbf{k},\sigma}, \tag{14}$$

where $\rho_{-\mathbf{q}}$ is the $-\mathbf{q}$ Fourier component of the dielectric particle density, and $v(q)=4\pi e^2/q^2$. The third term is the direct interaction between test electrons,

$$H_2=\tfrac{1}{2}\sum_{\mathbf{k}\mathbf{k}'\mathbf{q};\sigma\sigma'}v(q)a_{\mathbf{k}+\mathbf{q},\sigma}^\dagger a_{\mathbf{k}'-\mathbf{q},\sigma'}^\dagger a_{\mathbf{k}',\sigma'}a_{\mathbf{k},\sigma}. \tag{15}$$

Following Kittel, we construct a canonical transformation to decouple the two systems to lowest order. We shall consider the test electrons to be extremely dilute and assume that we can ignore H_2 in constructing the transformation, so that the eigenfunctions of the test electron system are plane waves. The transformation can be written

$$\tilde{H}=e^{-S}He^{S}=H+[H,S]+\tfrac{1}{2}[[H,S],S]+\cdots, \tag{16}$$

where S is an anti-Hermitian operator. We may remove H_1 to lowest order by requiring that

$$H_1+[H_0,S]=0. \tag{17}$$

The matrix elements of S may be found directly from (17) using the plane-wave representation for the test electrons and the $|n\rangle$ representation for the gas. Having decoupled the systems, we wish to average over the ground state of the dielectric. The effective Hamil-

[18] L. D. Landau, Zh. Eksperim. i Teor. Fiz. **30**, 1058 (1956) [English transl.: Soviet Phys.—JETP **3**, 920 (1956)].

[19] C. Kittel, *The Quantum Theory of Solids* (John Wiley & Sons, Inc., New York, 1963), p. 106.

[20] J. Lindhard, Kgl. Danske Videnskab. Selskab, Mat. Fys. Medd. **28**, No. 8 (1954).

[21] D. Bohm and D. Pines, Phys. Rev. **92**, 609 (1953).

[22] See Ref. 19, p. 151.

tonian for the screened test electrons is then given by

$$\langle 0|\tilde{H}|0\rangle=\sum_{\mathbf{k}\sigma}\epsilon_{\mathbf{k}}a_{\mathbf{k},\sigma}^{\dagger}a_{\mathbf{k},\sigma}+H_2+\tfrac{1}{2}\langle 0|[H_1,S]|0\rangle+\langle 0|[H_2,S]|0\rangle+0(v^3). \quad (18)$$

It is easily shown that the average value of $[H_2,S]$ is zero, since it contains one factor of $\rho_{\mathbf{q}}$ only. The average value of $[H_1,S]$ in the dielectric ground state contains an interaction between test electrons and a diagonal operator,

$$\begin{aligned}\tfrac{1}{2}\langle 0|[H_1,S]|0\rangle=&\tfrac{1}{4}\sum_{\mathbf{k}\mathbf{k}'\mathbf{q};\sigma\sigma'}\{v^2(q)a_{\mathbf{k}+\mathbf{q},\sigma}^{\dagger}a_{\mathbf{k}'-\mathbf{q},\sigma'}^{\dagger}a_{\mathbf{k}',\sigma'}a_{\mathbf{k},\sigma}\\&\times\sum_n|\langle n|\rho_{\mathbf{q}}|0\rangle|^2[(\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{k}+\mathbf{q}}-\omega_n)^{-1}-(\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{k}+\mathbf{q}}+\omega_n)^{-1}\\&+(\epsilon_{\mathbf{k}'}-\epsilon_{\mathbf{k}'-\mathbf{q}}-\omega_n)^{-1}-(\epsilon_{\mathbf{k}'}-\epsilon_{\mathbf{k}'-\mathbf{q}}+\omega_n)^{-1}]\}\\&+\sum_{\mathbf{k}\sigma}a_{\mathbf{k},\sigma}^{\dagger}a_{\mathbf{k},\sigma}\sum_{\mathbf{q}}v^2(q)\sum_n|\langle n|\rho_{\mathbf{q}}|0\rangle|^2(\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{k}-\mathbf{q}}-\omega_n)^{-1}. \quad (19)\end{aligned}$$

It is now necessary to consider the fact that (19) is not a well-defined expression because the eigenvalues ω_n form a continuum, and the energy denominators will, in general, vanish somewhere in the range of the n sums. Since the eigenstates $|n\rangle$ are unknown, in fact, and since their degeneracy is infinite at any energy, this question cannot be decided by recourse to exact expressions as may be done to decide similar problems which arise in one-particle scattering theory. For lack of a better alternative, we will argue as follows: The dressed electron states we wish to describe are to be approximately stationary, neither growing nor decaying in time. For this to be true, the bare test particles must be scattered out of and back into their initial state at the same rate by the virtual excitation and de-excitation of the dielectric. This process suggests the analogy of standing wave states in one-particle scattering theory, which are superpositions of incoming and outgoing wave scattering solutions. The integrals over singular energy denominators are treated as principal values in the expansion of these standing wave solutions, and we shall do the same. It should be noted that it is not this approximation, but the fact that we average over the ground state of the dielectric that forbids test electron-dielctric energy exchange and requires the test electron effective Hamiltonian to be Hermitian.

As it stands, (19) is of little use since it contains unknown exact energies and matrix elements. However, this same combination occurs in an exact eigenstate treatment of the electron gas response to a time-dependent external potential as

$$\epsilon^{-1}(q,\omega)-1=v(q)\sum_n|\langle n|\rho_q|0\rangle|^2[(\omega-\omega_n+i\eta)^{-1}-(\omega+\omega_n+i\eta)^{-1}], \quad (20)$$

where $\epsilon(q,\omega)$ is the retarded dielectric function and η is a positive infinitesimal.[23] Utilizing the well-known symbolic identity

$$1/(x\pm i\eta)=P/x\mp i\pi\delta(x), \quad (21)$$

where P denotes the Cauchy principal value, we can easily show that

$$v(q)\sum_n|\langle n|\rho_q|0\rangle|^2(\omega-\omega_n)^{-1}=\pi^{-1}P\int_0^{\infty}dt(\omega-t)^{-1}|\mathrm{Im}\epsilon^{-1}(q,t)|. \quad (22)$$

Relations (20) and (22) enable us to identify all the unknown elements of (19) in terms of the electron gas dielectric function, which can be calculated approximately. It is found that the interaction term in (19) contains a long-range part which exactly cancels the direct Coulomb interaction between the test electrons, H_2, and that the remainder is short range.

If we now apply the test electron effective Hamiltonian to a Fermi sea of quasiparticles, and remove the diagonal exchange portion from the two-particle interaction by expressing the Hamiltonian in terms of normal products,[24] we obtain

$$\begin{aligned}H_{QP}=&\sum_{\mathbf{k}\sigma}\Big\{:a_{\mathbf{k},\sigma}^{\dagger}a_{\mathbf{k},\sigma}:\Big[\epsilon_{\mathbf{k}}-\sum_{\mathbf{q}}v(q)n_{\mathbf{k}-\mathbf{q}}\,\mathrm{Re}\epsilon^{-1}(q,\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{k}-\mathbf{q}})\\&+\sum_{\mathbf{q}}v(q)\pi^{-1}P\int_0^{\infty}dt(\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{k}-\mathbf{q}}-t)^{-1}|\mathrm{Im}\epsilon^{-1}(q,t)|\Big]\Big\}\\&+\tfrac{1}{4}\sum_{\mathbf{k}\mathbf{k}'\mathbf{q};\sigma\sigma'}\{:a_{\mathbf{k}+\mathbf{q},\sigma}^{\dagger}a_{\mathbf{k}'-\mathbf{q},\sigma'}^{\dagger}a_{\mathbf{k}',\sigma'}a_{\mathbf{k},\sigma}:v(q)\\&\times[\mathrm{Re}\epsilon^{-1}(q,\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{k}-\mathbf{q}})+\mathrm{Re}\epsilon^{-1}(q,\epsilon_{\mathbf{k}'}-\epsilon_{\mathbf{k}'-\mathbf{q}})]\}. \quad (23)\end{aligned}$$

The self-consistent-field approximation to the dielectric function[20] is then used,

$$\epsilon(q,\omega)=1+2v(q)\sum_{\mathbf{k}}\frac{n_{\mathbf{k}}-n_{\mathbf{k}+\mathbf{q}}}{\epsilon_{\mathbf{k}+\mathbf{q}}-\epsilon_{\mathbf{k}}-\omega-i\eta}. \quad (24)$$

Since (23) is to be employed at metallic densities, exchange corrections to (24) are undoubtedly significant for large q.[2] However, it is the small q interactions that are of most importance in the question of the SDW instability.

An alternative derivation of the test electron effective Hamiltonian was carried out in which the transformation generator S was found by solving (17) approximately as an operator equation instead of introducing the eigenstate representation of H_d. The key step in this approach was a form of the random-phase approxima-

[23] P. Nozières and D. Pines, Nuovo Cimento **9**, 470 (1958).

[24] The normal product of a set of field operators is indicated by enclosing the operators between colons. It is an ordered product defined in terms of some particular vacuum state (in this case the Fermi sphere) so that operators which annihilate excitations of the vacuum stand to the right. For Wick's theorem relating normal products to ordinary products, see N. Bogoliubov and D. Shirkov, *Introduction to the Theory of Quantized Fields*, translated by G. Volkoff (Interscience Publishers Inc., New York, 1959), p. 159.

tion,[21,2] replacing pairs of operators in a four operator expression by their expectation value. It was necessary to take principal values at two stages in this derivation, both corresponding to degenerate-state matrix elements of (17). This derivation yielded a form similar to (23) for H_{QP} but with $\mathrm{Re}(v/\epsilon)$ replaced by $v/\mathrm{Re}\epsilon$ in the screened interaction, and some corresponding changes in the diagonal part (the self-energy). The self-consistent field approximation to ϵ occurred directly in this second derivation.

In a treatment of the interaction between "minority carriers" (similar to our test electrons) in the presence of an electron gas, Nozières and Pines obtained a screened interaction similar to our second result[25] using the Bohm and Pines collective coordinate method.[21] In a later paper, Nozières and Pines derived a screened interaction between two classical test charges similar to our first result.[23] They argue that this $[\mathrm{Re}(v/\epsilon)]$ is more correct than their earlier result $(v/\mathrm{Re}\epsilon)$. The quasiparticle energy given by our first method is identical to that obtained using the simplest self-energy diagram with the screened interaction in the Green's-function formalism, an approximation first used by Quinn and Ferrell.[26] This equivalence is demonstrated in the Appendix.

Despite these arguments, it was not entirely clear (to us) that the retarded dielectric function should appear in a quasiparticle theory designed to treat a static problem. The damped screened interaction, $\mathrm{Re}(v/\epsilon)$, and the undamped, $v/\mathrm{Re}\epsilon$, display considerable differences, the latter being singular for electrons near the Fermi surface. Therefore it was decided to carry out the susceptibility calculation using both forms.

4. SOLUTION OF THE SUSCEPTIBILITY INTEGRAL EQUATION

The same linearized self-consistent field technique described in Sec. 2 can be used with H_{QP} to find $\chi(Q)$ for the quasiparticle gas. It can be verified that the perturbing magnetic field interacts with the quasiparticles as if they were bare electrons by applying the canonical transformation (16) to (2), and observing that the average value in the dielectric ground state of the first-order term vanishes. Physically, this reflects the fact that the screening charge is not coupled to the spin of the screened electron in our approximation. It is more convenient to use a momentum representation throughout in this $\chi(Q)$ calculation rather than a form such as (6), since the interaction in H_{QP} is velocity-dependent. Because the physics is the same, however, we will not write out this calculation. The integral equation for the amplitude of the exchange potential is

$$U(\mathbf{k})=1+\tfrac{1}{2}\sum_{\mathbf{k}'}\frac{n_{\mathbf{k}'-\mathbf{Q}/2}-n_{\mathbf{k}'+\mathbf{Q}/2}}{E_{\mathbf{k}'+\mathbf{Q}/2}-E_{\mathbf{k}'-\mathbf{Q}/2}}U(\mathbf{k}') \times[V(\mathbf{k}-\mathbf{k}',\mathbf{k}'+\mathbf{Q}/2)+V(\mathbf{k}'-\mathbf{k},\mathbf{k}-\mathbf{Q}/2)], \quad (25)$$

and the susceptibility is given by

$$\chi(Q)=2\mu_B^2\sum_{\mathbf{k}}\frac{n_{\mathbf{k}-\mathbf{Q}/2}-n_{\mathbf{k}+\mathbf{Q}/2}}{E_{\mathbf{k}+\mathbf{Q}/2}-E_{\mathbf{k}-\mathbf{Q}/2}}U(\mathbf{k}). \quad (26)$$

In (25) and (26), E_k is the bracketed expression in the diagonal part of (23), and

$$V(\mathbf{q},\mathbf{k})=\mathrm{Re}v(q)\epsilon^{-1}(q,\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{k}+\mathbf{q}}). \quad (27)$$

For the case of the alternative derivation of H_{QP}, the right side of (27) would have the undamped form of the interaction, and E_k would be appropriately modified. It is easily seen that (25) and (26) reduce to the result of Sec. 2 when $\epsilon(q,\omega)$ is set equal to unity, and E_k to the one-electron HF energy.

One assumption underlying this entire treatment is that changes in the dielectric function caused by the infinitesimal applied magnetic field produce only higher order corrections to the magnetization than the linear contribution retained. This would obviously be true if all the one-electron wave functions were perturbed only an infinitesimal amount. However, those for which $\epsilon_{\mathbf{k}}=\epsilon_{\mathbf{k}+\mathbf{Q}}$ are perturbed a finite amount, and we are forced to assume that the number of such states is not significant. It is not possible to prove this point within the context of the present treatment.

In considering the means of solution of (25), we decided to use an effective mass approximation for E_k, $E_k=k^2/2m^*$, choosing m^* it give the correct density of states at the Fermi surface. This approximation is exact at small Q, and should not modify any effects of the SDW instability at large Q, since these involve states near the Fermi surface. E_k is evaluated numerically at several points near k_F to obtain m^* for each density of interest.

It can be shown that $U(\mathbf{k})=U(-\mathbf{k})$, enabling the sum to be "folded" into half the volume. Changing from summation to integration and using the dimensionless variables $\mathbf{q}=\mathbf{Q}/k_F$, $\mathbf{x}=\mathbf{k}/k_F$, and $\mathbf{x}'=\mathbf{k}'/k_F$, the equation to be solved is

$$U(\mathbf{x})=1+(m^*/4\pi^2ma_0k_F)\int d^3x'\{n_{\mathbf{x}'-\mathbf{q}/2}(1-n_{\mathbf{x}'+\mathbf{q}/2})(\mathbf{x}'\cdot\mathbf{q})^{-1}\mathrm{Re}[|\mathbf{x}-\mathbf{x}'|^{-2}\epsilon^{-1}(|\mathbf{x}-\mathbf{x}'|,x^2-x'^2-\mathbf{q}\cdot(\mathbf{x}-\mathbf{x}')) +|\mathbf{x}-\mathbf{x}'|^{-2}\epsilon^{-1}(|\mathbf{x}+\mathbf{x}'|,x^2-x'^2+\mathbf{q}\cdot(\mathbf{x}-\mathbf{x}'))+|\mathbf{x}+\mathbf{x}'|^{-2}\epsilon^{-1}(|\mathbf{x}+\mathbf{x}'|,x^2-x'^2-\mathbf{q}\cdot(\mathbf{x}+\mathbf{x}')) +|\mathbf{x}+\mathbf{x}'|^{-2}\epsilon^{-1}(|\mathbf{x}+\mathbf{x}'|,x^2-x'^2+\mathbf{q}\cdot(\mathbf{x}+\mathbf{x}'))]U(\mathbf{x}')\}, \quad (28)$$

[25] P. Nozières and D. Pines, Phys. Rev. **109**, 762 (1958).
[26] J. Quinn and R. Ferrell, Phys. Rev. **112**, 812 (1958).

where a_0 is the first Bohr radius. In terms of these same variables, the susceptibility is

$$\chi(Q)=(\chi_P m^*/2\pi m)\int d^3x\, n_{\mathbf{x}-\mathbf{q}/2}(1-n_{\mathbf{x}+\mathbf{q}/2})U(\mathbf{x})/\mathbf{x}\cdot\mathbf{q}\,, \tag{29}$$

where $\chi_P=3n\mu_B^2/2E_F$ is the Pauli susceptibility, n being the electron density and $E_F=k_F^2/2m$.

The dielectric function (24) can be evaluated analytically, but is sufficiently complicated that the analytic solution of (28) was not considered. It can be shown from (28) that $U(\mathbf{k})$ possesses axial symmetry about $\mathbf{Q}$. Therefore only a two-dimensional integral equation must be solved, and this was considered a feasible numerical calculation. Equation (28) qualifies as an inhomogeneous Fredholm equation of the second kind if a small amount of damping of the plasma zero of $\epsilon(q,\omega)$ is added. As such, it possesses unique solutions for all but isolated values of m^*/a_0k_F (Q being fixed). It seemed probable that the iterative expansion of U would not converge when an instability existed, so this method was rejected. Instead, it proved practical to use the Fredholm expansion[27,28] by exploiting the fact that only χ, a particular integral of the unknown function, was desired rather than the unknown function itself.

Before discussing the method of solution, we will describe the numerical method used to perform integrals such as occur in (28) and (29), since this will lead to an economical notation. Spherical coordinates were chosen, with the z axis parallel to $\mathbf{Q}$, since these will concentrate mesh points in the region where the energy denominator is small and where presumably U will be large. A mesh of points in a plane containing the z axis is chosen, a typical example being shown in Fig. 1, and numbered consecutively. A weighting factor w_j containing the Jacobian, the energy denominator and numerical weighting factors[29] is assigned to each point (θ_j,x_j). In terms of this scheme, (28) can be represented as

$$U_i=1+\sum_j K_{ij}w_jU_j\,, \tag{30}$$

where $U_i=U(\theta_i,x_i)$, and

$$K_{ij}=\int_0^{2\pi} d\varphi\, K(\theta_i,x_i;\theta_j,x_j;\varphi)\,. \tag{31}$$

$K(\mathbf{x};\mathbf{x}')$ is the bracketed expression in (28), which depends on the polar angles of $\mathbf{x}$ and $\mathbf{x}'$ only through their difference φ, and is symmetric under the interchange of $\mathbf{x}$ and $\mathbf{x}'$.

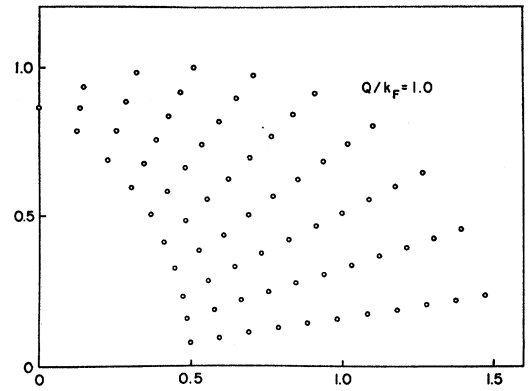

FIG. 1. A typical mesh used in numerical integrations performed in solving the susceptibility integral equation. The abscissa is the z axis, and the ordinate is any line in the x-y plane.

Since it is desirable to deal with a symmetric kernel, the substitutions

$$\begin{aligned} v_j&=(w_j)^{1/2}\,,\\ K_{ij}'&=(w_i)^{1/2}K_{ij}(w_j)^{1/2}\,,\\ g_i&=U_i(w_i)^{1/2}\,, \end{aligned} \tag{32}$$

were made in (30), giving

$$g_i=v_i+\sum_j K_{ij}'g_j\,. \tag{33}$$

These same steps can be carried out for (29), giving

$$\chi=\text{const}\sum_i v_ig_i\,. \tag{34}$$

It is now possible to explain the Fredholm method and its application to this problem very simply. Rewriting (33) without the indices, and introducing the "interaction strength" parameter λ which will eventually be set equal to unity,

$$g=v+\lambda K'g\,. \tag{35}$$

[This might be regarded as an abstract representation of (28) instead of a result of the numerical integration scheme.] The solution may be formally written

$$g=(1-\lambda K')^{-1}v \tag{36}$$

and the susceptibility

$$\chi=\text{const}\,\tilde{v}(1-\lambda K')^{-1}v\,, \tag{37}$$

where $\tilde{v}$ indicates the transpose of the one-column matrix v. The resolvent kernel (or Green's function) $(1-\lambda K')^{-1}$ for (35) is known to exist for all but certain isolated values of λ, the eigenvalues of the homogeneous equation, which are real in this case since K' is symmetric. The iterative solution corresponds to an expansion of $(1-\lambda K')^{-1}$ in a power series in λ, whose radius of convergence is determined by the eigenvalue

[27] R. Courant and D. Hilbert, *Methods of Mathematical Physics* (Interscience Publishers Inc., New York, 1953), Vol. 1, p. 142.

[28] P. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill Book Company, New York, 1953) Vol. 2, p. 1018.

[29] A numerical integration scheme was employed in which first the x and then the θ integration is carried out, using one-dimensional parabolic interpolation for each, but overlapping the parabolas so that the interior points are weighted equally and curvature corrections occur at the ends of the range only. The "numerical weighting factors" contain these curvature factors and factors proportional to the spacing of the mesh points.

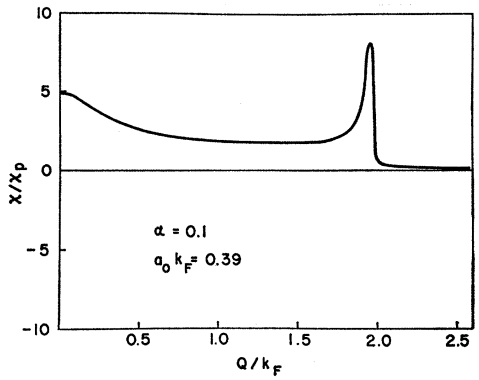

FIG. 2. Numerical susceptibility results using the interaction (46) showing stable but anomalous behavior.

closest to the origin of the complex λ plane. The Fredholm solution corresponds to writing

$$\frac{1}{(1-\lambda K')}=\frac{\varphi(\lambda)/(1-\lambda K')}{\varphi(\lambda)}, \tag{38}$$

where φ is a scalar function. If φ is an entire function with zeros of the proper order at each eigenvalue, the numerator and denominator on the right in (38) will be entire functions, and thus possess convergent power series expansions for all finite λ. One conveneint way to choose such a φ is to have it satisfy

$$\frac{d}{d\lambda}\ln(\varphi(\lambda))=\mathrm{tr}[-K'/(1-\lambda K')], \tag{39}$$

where tr denotes trace. The desired power series expansion for φ is found to be[28]

$$\varphi(\lambda)=\sum_{n=0}^{\infty}a_n\lambda^n, \tag{40}$$

where $a_0=1$, and

$$a_n=\frac{-1}{n!}\begin{vmatrix} 1 & 0 & 0 & \cdots & 0 & \kappa_1 \\ \kappa_1 & 2 & 0 & & 0 & \kappa_2 \\ \kappa_2 & \kappa_1 & 3 & & 0 & \kappa_3 \\ \kappa_3 & \kappa_2 & \kappa_1 & & 0 & \kappa_4 \\ \vdots & & & & & \\ \kappa_{n-1} & \kappa_{n-2} & \kappa_{n-3} & & \kappa_1 & \kappa_n \end{vmatrix}. \tag{41}$$

In (41), κ_n is the trace of the nth power of K'. The expansion of the numerator in (38) is

$$\frac{\varphi(\lambda)}{1-\lambda K'}=\sum_{n=0}^{\infty}B_n\lambda^n, \tag{42}$$

where the B_n are matrices, B_0 being the unit matrix I, and

$$B_n=(K')^n+a_1(K')^{n-1}+\cdots+a_{n-1}K'+a_nI. \tag{43}$$

The series (42) would be very difficult to compute; however, we do not need the matrix for (38), but merely its "expectation value in the state v." The susceptibility can be expanded

$$\chi=\mathrm{const}\Big(\sum_{n=0}^{\infty}a_n\lambda^n/\sum_{n=0}^{\infty}b_n\lambda^n\Big), \tag{44}$$

where

$$\begin{aligned} b_n&=\sum_{j=0}^{n}a_jc_{n-j}, \\ c_n&=\tilde{v}(K')^nv, \end{aligned} \tag{45}$$

as may be seen from (37) and (43). The quantities κ_n and c_n may be computed quite easily once the matrix K' is known.

In practice, the coefficients a_n and b_n converge quite rapidly, and if we define the Nth Fredholm approximant to χ as the expression given by (44) with the sums terminated at $n=N$, N usually need not be too large. The entire procedure described above must be performed for each value of Q and a_0k_F (and its corresponding effective mass) for the dynamically screened interaction. For the "statically screened" interaction $4\pi e^2/(q^2+\alpha^2k_F^2)$, however, it is possible for each Q and α to execute the entire solution for just one value of a_0k_F, and then use (44) with $\lambda=m^{*\prime}a_0k_F/a_0k_F'm^*$ for each other a_0k_F' desired, instead of setting λ equal to unity. For this reason, it was practical to compute $\chi(Q)$ for a wide range of α and a_0k_F with this interaction. In addition, the φ integration in (31) can be performed analytically in this case.

The procedure described in this section was programmed for execution on a Philco 212 computer. The program was designed to utilize a maximum mesh of 130 points, and to compute at most the 20th Fredholm approximant. The most lengthy stage of each execution of the entire computation was finding the matrix K'.

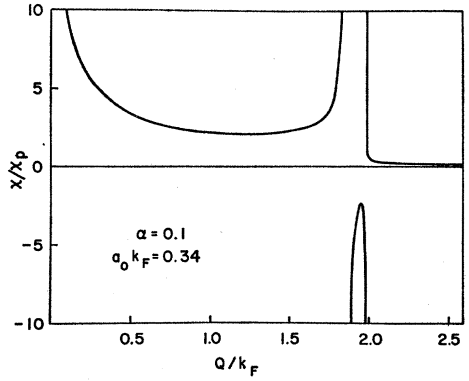

FIG. 3. Numerical susceptibility results using the interaction (46) showing an antiferromagnetic instability. At small Q, the curve bends over and hits the ordinate at $\chi/\chi_P=12$.

5. SUSCEPTIBILITY FOR A STATICALLY SCREENED INTERACTION

Before carrying out the solution of (28), $\chi(Q)$ was calculated using the theory of Sec. 2 and the interaction

$$v(q)=4\pi e^2/(q^2+\alpha^2 k_F^2). \tag{46}$$

This "statically screened" interaction was not intended to represent the electron gas, but rather to provide a simple adjustable-range interaction with which to develop an understanding of the classes of behavior to be expected from $\chi(Q)$ results. The screening parameter is chosen to be a fixed fraction of k_F rather than a constant, so that changing k_F simply changes the relative importance of potential and kinetic energy, and not the "packing" of the particles. The Thomas-Fermi approximation for the screened electron interaction corresponds to[19]

$$\alpha=[4\pi/a_0 k_F]^{1/2}. \tag{47}$$

The effective mass approximation for E_k [given by (7) in this case] can be evaluated analytically using (46), yielding

$$(m^*/m)=\{1-(1/2\pi a_0 k_F)[4-(2+\alpha^2)\ln(1+4/\alpha^2)]\}^{-1}. \tag{48}$$

In addition, the integral equation may be solved exactly in the small Q limit (ferromagnetic deformation), in which the effective mass approximation is exact. The critical density for the onset of ferromagnetic instability (as the density is decreased) is

$$a_0 k_F=(1/\pi)[1-(\alpha^2/4)\ln(1+4/\alpha^2)]. \tag{49}$$

This can be verified by examining the dependence of the HF energy on an infinitesimal number of flipped spins, an approach which appears different but in fact involves the same physical picture as the small-Q limit approach. It should be noted that in the $\alpha=0$ limit (bare Coulomb interactions), (49) predicts $a_0 k_F=1/\pi$ as the critical value. Bloch, however, derived the critical value $a_0 k_F\approx 1.1/\pi$ by comparing the energies of the unpolarized and fully polarized states.[30] Thus for $a_0 k_F$ between these values, the paramagnetic state is stable with respect to infinitesimal ferromagnetic deformations, but is in fact ferromagnetically unstable (in the HF approximation). Equation (49) also provided a useful and nontrivial check on the numerical methods discussed in the last section.

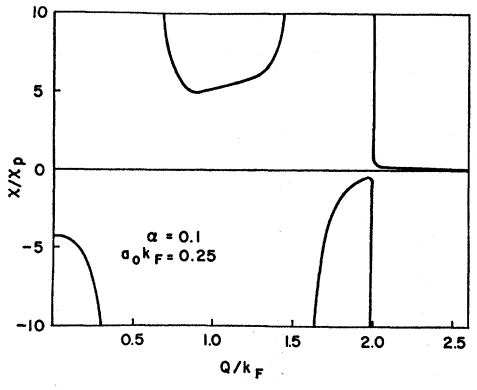

FIG. 4. Numerical susceptibility results using the interaction (46) showing disjoint ferromagnetic and antiferromagnetic unstable regions.

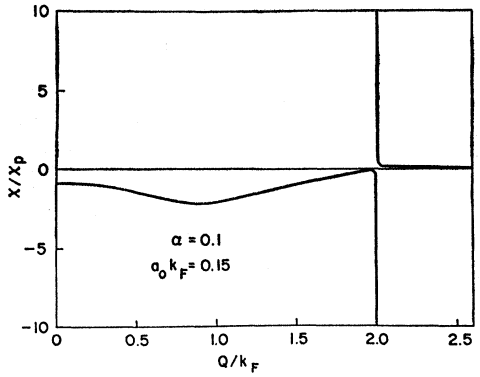

FIG. 5. Numerical susceptibility results using the interaction (46) showing a single unstable region with instability maxima at $Q=0$ and near $Q=2k_F$.

The only other limit which can be investigated analytically is that of large α, that is, delta function interactions. Wolff gave the results for this case,[9] and we shall describe them briefly for completeness. For weak δ interactions, $\chi(Q)$ is a monotonically decreasing function of Q, but enhanced in magnitude over the χ of the noninteracting gas. For the strength greater than a critical value, χ has a negative region peaked at $Q=0$, a singularity, and is positive and monotonically decreasing above the singularity. From the discussion in the introduction, we would infer that such behavior indicates a maximum instability for $Q=0$ deformations.

The $\chi(Q)$ results for a rather long-range case, $\alpha=0.1$ are shown in Figs. 2–5. At high densities, $\chi(Q)$ shows no interesting structure. As $a_0 k_F$ is descreased, a peak develops near $Q=2k_F$ (Fig. 2). Further decrease produces a negative region peaked near $Q=2k_F$, and separated by singularities from the low-Q and high-Q positive regions (Fig. 3). This indicates that the gas is antiferromagnetically unstable, the Q of maximum instability occurring at the peak of the negative region. At still lower densities ferromagnetic and antiferromagnetic unstable regions occur (Fig. 4), and finally the intermediate-Q stable region disappears (Fig. 5).

Investigations were carried out using the interaction (46) for $\alpha=0.1$, 0.2, 0.3, 0.4, 0.6, 1.0, and 2.0. The results in these cases displayed the same qualitative forms of behavior as have been discussed. For shorter range interactions, however, the ferromagnetic instability seemed dominant.

For $\alpha=0.3$, for example, the high-density results were monotonically decreasing. As the density was lowered,

[30] F. Bloch, Z. Physik **57**, 545 (1929).

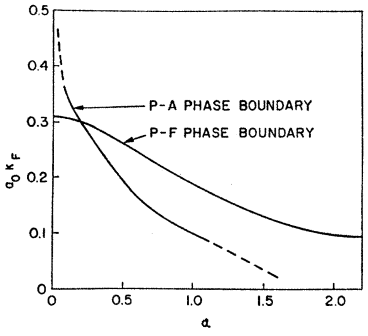

FIG. 6. Diagram indicating the values of $a_0 k_F$ and α for which instabilities are first observed. P-A stands for paramagnetic-antiferromagnetic and P-F for paramagnetic-ferromagnetic.

a negative region first appeared near $Q=0$ and peaked there, and a sharp peak formed in the positive region near $2k_F$. At a lower density, peaked negative regions were present around 0 and $2k_F$, with a stable positive region between. Finally at sufficiently low densities this stable region vanished, and the single negative portion of the curve continued to display peaks at 0 and near $2k_F$.

For shorter range interactions, two distinct negative regions no longer appeared. Instead, the negative region initially formed around $Q=0$, and then moved out toward $2k_F$ and formed a second peak as the density was lowered. The shorter the range the lower the density at which such a peak formed. For the shortest range interaction investigated, $\alpha=2.0$, it was no longer possible to discern with certainty whether or not such peaking occurred at large wave vector. The limiting behavior, of course, is that of the δ function, where only the $Q=0$ peak exists in the negative region.

The results of this investigation are best summarized through a type of "phase diagram," which is shown in Fig. 6. Each point on this diagram represents a particular value of α and $a_0 k_F$. The location of the point relative to the two lines labeled "phase boundaries" indicates the qualitative nature of the susceptibility curve for these values. Toward the upper right, the

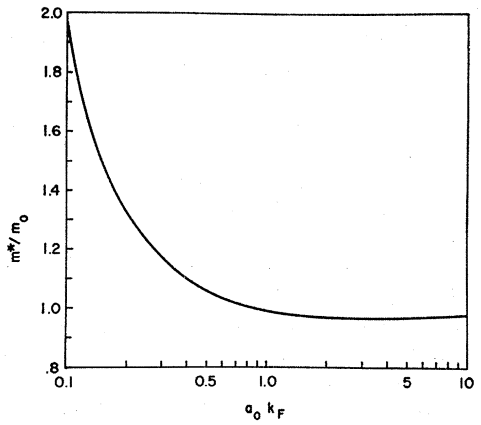

FIG. 7. The electron quasiparticle effective mass, chosen to give the correct Fermi surface density of states, as a function of density.

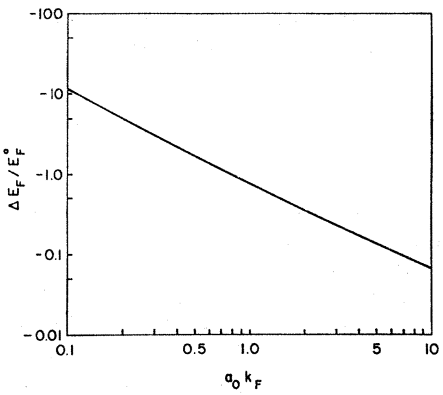

FIG. 8. The electron quasiparticle self-energy at the Fermi surface as a function of density. E_F^0 is the unperturbed Fermi energy, $k_F^2/2m$.

paramagnetic state is stable. Below the P-A (paramagnetic-antiferromagnetic) boundary, the paramagnetic state is unstable and the negative portion of the χ curve shows a peak toward $2k_F$. The numerical accuracy obtained was not sufficient to decide unambiguously whether this curve should terminate on the abscissa or approach it asymptotically. For small α, the curve is shown to approach the ordinate asymptotically since the HF antiferromagnetic instability is present at all densities.[1] The P-F (paramagnetic-ferromagnetic) boundary is based on the analytic result (49), and the paramagnetic state is unstable relative to ferromagnetic deformations below it. This plot cannot be regarded as a phase diagram in the true sense since it only reflects the instability of the paramagnetic state relative to infinitesimal deformations. The relative stabilities of the ferromagnetic and antiferromagnetic states in the area near the lower left-hand corner cannot be compared by this method. Also, as shown by example earlier in this section, the consideration of infinitesimal deformations only is not a sufficient criterion to establish the stability of a state.

It may be seen from (47) and Fig. 6 that the Thomas-Fermi screened interaction would not predict an

TABLE I. The self-energy and effective mass of a dressed electron quasiparticle at the Fermi surface.

$a_0 k_F$	m^*/m_0	$\Delta E_F/(k_F^2/2m)$
0.1	1.96	−11.4
0.2	1.32	−4.97
0.3	1.17	−3.08
0.4	1.10	−2.20
0.5	1.06	−1.70
0.6	1.03	−1.38
0.8	1.005	−0.995
1.0	0.990	−0.774
1.5	0.973	−0.494
2.0	0.967	−0.361
3.0	0.965	−0.233
5.0	0.967	−0.136
10.0	0.974	−0.0662

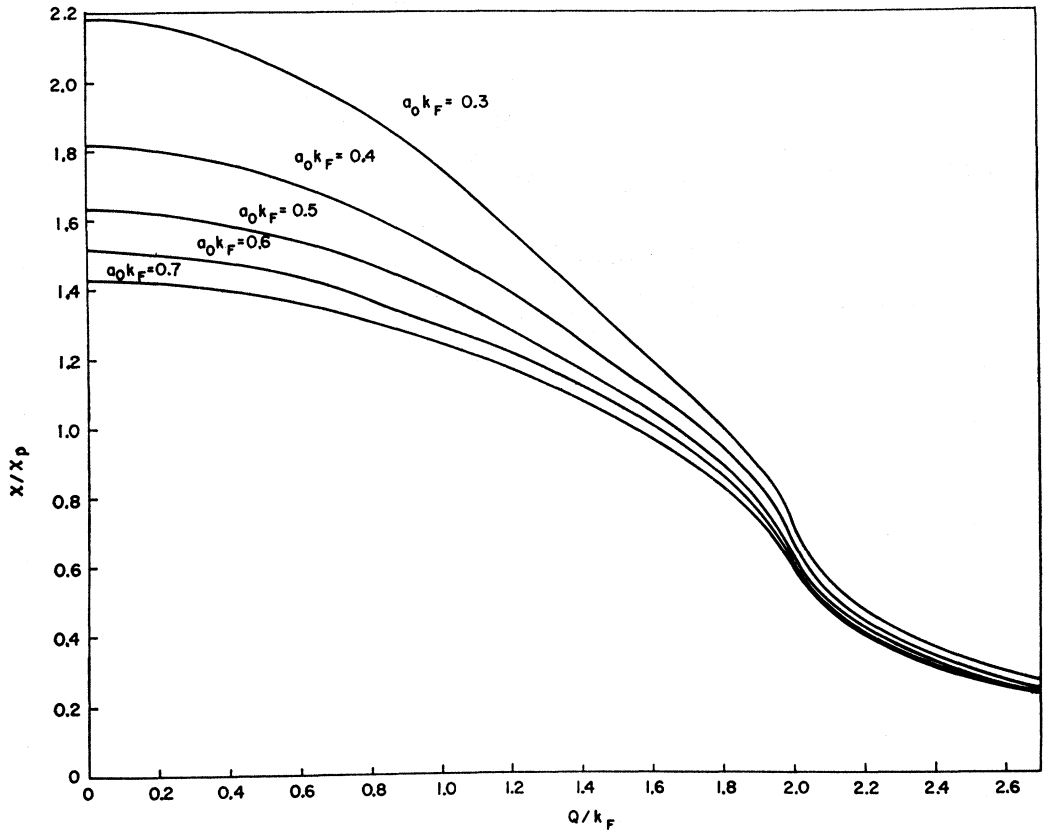

FIG. 9. The electron-gas susceptibility in the metallic density region calculated using the damped dynamically screened interaction. The vertical scale is in units of the Pauli susceptibility.

antiferromagnetic instability for the electron gas at metallic densities.

We note that it was necessary to go to the fifteenth Fredholm approximant for the small α cases. Extensive tests indicated an over-all accuracy of the numerical computation of about 1%.

6. THE ELECTRON-GAS SUSCEPTIBILITY

A necessary preliminary to the actual calculation of the susceptibility within the quasiparticle framework is the evaluation of the quasiparticle energy-momentum relation. The form derived along with the damped screened interaction, given by the bracketed coefficient of the diagonal term in (23), was evaluated numerically in the vicinity of $k=k_F$ for a number of densities spanning the metallic range.[31] The resulting values of the effective mass and the self-energy of an electron at the Fermi surface are shown in Figs. 7 and 8 and in Table I. The quasiparticle mass increases rapidly at low densities, but is close to the bare electron mass in the metallic region. In the high-density region, the quasiparticle mass approaches the electron mass in a manner similar to the high-density approximation to the same mathematical form calculated by Quinn and Ferrell.[26] The energy shift at the Fermi surface is large in the metallic region, of the order of the kinetic energy. Its magnitude, which is almost a straight line on the log-log plot shown, varies approximately as a_0k_F to the -1.1 power. Thus the (dimensionless) Fermi energy shift comes close to being proportional to the (dimensionless) interaction strength, which is reasonable but unexpectedly simple. The self-energy expression derived with the quasiparticle Hamiltonian having undamped screened interactions was not evaluated, since an effective mass close to unity was anticipated on the basis of the previous calculation.

The susceptibility calculated using the damped screened interaction is shown in Fig. 9 for a series of densities spanning the metallic range. The corresponding results using the undamped screened interaction (but effective masses from Fig. 7) are shown in Fig. 10. The results computed using both methods are compared with the noninteracting electron-gas susceptibility in Fig. 11 at one density well above the metallic range, where the quantitative errors introduced by the use of the self-consistent-field dielectric function should be

[31] The dimensionless density parameter a_0k_F, where a_0 is the first Bohr radius, proved more convenient in this work than the customary r_s. The two are related by $a_0k_F=(9\pi/4)^{1/3}r_s^{-1}$. The metallic density range is roughly $0.3<a_0k_F<0.7$.

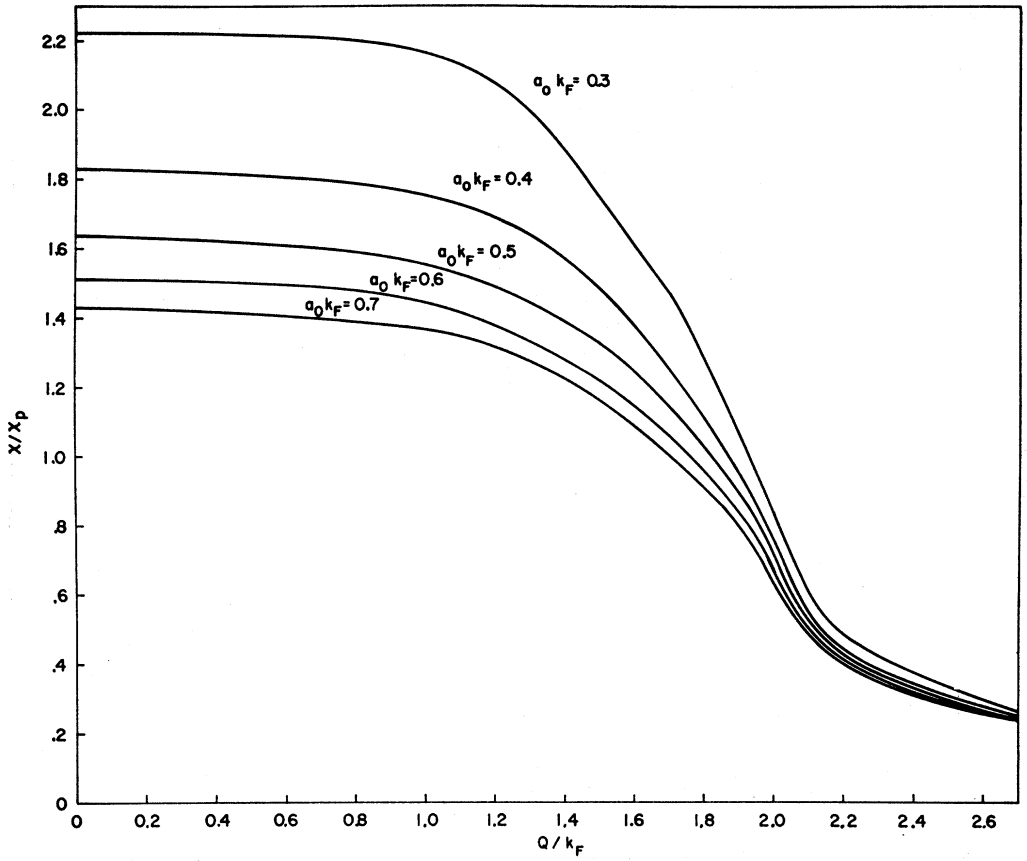

FIG. 10. The electron-gas susceptibility in the metallic density region calculated using the undamped dynamically screened interaction. The vertical scale is in units of the Pauli susceptibility.

small. It is seen that in all cases the susceptibility is positive and monotonically decreasing. The electron interactions have no significant qualitative effect, and simply enhance the magnitude of χ. It should be noted that the vertical scale in these figures is in units of χ_P,

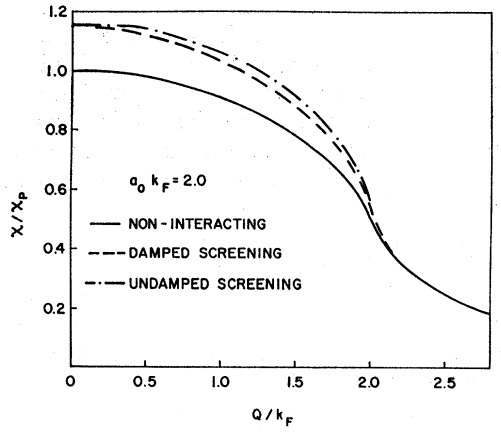

FIG. 11. The electron gas susceptibility for $a_0 k_F = 2$, computed using both forms of the dynamically screened interaction and compared to the noninteracting gas susceptibility.

the Pauli susceptibility. Since $\chi_P = 3n\mu_B^2/2E_F$, where n is the electron density, μ_B the Bohr magneton, and $E_F = k_F^2/2m$, the scale in absolute units is different for each curve, and the graphs show the relative enhancement of χ caused by the interaction at each density.

Considering the the complexity of the dynamically screened interaction, it was surprising that no more complex structure was obtained in the χ curves, and that the use of the damped or undamped form made so little difference. It was also observed that the Fredholm approximants converged rapidly, the fourth usually being within the estimated over-all numerical accuracy of 1%. This suggested that the self-consistent field U in (28) was not a rapidly varying function, in contrast with the case of the long-range interaction examples in Sec. 5, where the lower order Fredholm terms did not converge, and it is expected from related calculations that U should vary rapidly.[1] U being a slowly varying function would account for much of the detail of the dynamically screened interaction being "averaged out" in the integral equation. In fact, a fair portion of this averaging may take place in the angular integration (31) arising simply from the axial symmetry of U.

TABLE II. Calculated zero wave-vector susceptibilities in the metallic density region.

a_0k_F	χ/χ_P
0.3	2.18
0.4	1.81
0.5	1.62
0.6	1.50
0.7	1.42

In carrying out the numerical integrations, a small constant imaginary term ($0.1i$) was added to $\epsilon(q,\omega)$ where ϵ was real as an expeditious way of dealing with the plasma pole. In addition, a similar device was used in the undamped screening case (so that it was in fact "slightly damped"). It was shown in Sec. 5 that a singular interaction is not necessary to obtain structured $\chi(Q)$ curves and an antiferromagnetic instability. Therefore it is not expected that a more careful treatment of the relatively weak singularities in the dynamic screening calculation would change the results.

The dependence of the uniform susceptibility $\chi(0)$ on density has been calculated by several authors.[13–15] These treatments, based on modern calculations of the correlation energy, find the change in the total energy of the electron gas caused by an infinitesimal uniform polarization. This makes it extremely difficult to compare the approximations made in these treatments with those of our Q-dependent approach. However, calculated values of $\chi(0)$ may be compared with observed Knight-shift results. Since all the calculations are based on the free-electron gas model, a difficulty attending this comparison is that of including band structure. Following Pines,[13] all the other calculations incorporated the band-structure effective mass in the kinetic energy contribution to the polarization, and gave the other terms their free-electron gas value. While Pines' arguments are plausible, the separation seems a somewhat arbitrary one on which to base quantiative comparisons, especially since this approximation makes the susceptibility strongly dependent on the effective mass. Lacking quantitative arguments on how to include band structure effective masses in the present theory, we have chosen to compare the theoretical results with each other and with experimental results for the alkali metals on a strictly free-electron gas picture.

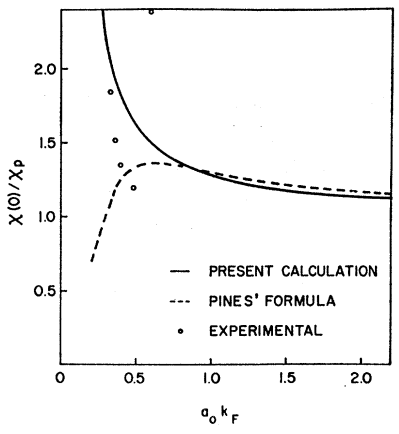

FIG. 12. The ratio of the paramagnetic susceptibility of the interacting electron gas to that of the noninteracting electron gas, compared to Pines' theoretical result and experimental Knight-shift results for Li, Na, K, Rb, and Cs (right to left).

TABLE III. Knight-shift data used in Fig. 12.

Metal	K^a ($\times10^{-3}$)	$P_F{}^a$	$a_0k_F{}^b$	χ/χ_P
Li	0.249	0.11	0.593	2.40
Na	1.13	0.664	0.482	1.20
K	2.48	0.862	0.395	1.35
Rb	6.53	1.76	0.362	1.52
Cs	14.9	2.89	0.332	1.84

[a] Ref. 32.
[b] From Pines' value for r_s, Ref. 13.

The Knight shift, K is related to the susceptibility (of s-band electrons) by

$$K=(8\pi/3)\chi P_F, \tag{50}$$

where P_F is the squared magnitude of the conduction electron wave function at the nucleus, averaged over the Fermi surface. Experimental values for K and theoretical values for P_F were taken from Muto *et al.*,[32] and the reader is referred to their paper for the original sources. The values of χ/χ_P obtained from our theory, from Pines' theory, and from the Knight-shift data are plotted as a function of a_0k_F in Fig. 12. Plotting this particular quantity reveals the discrepancies most clearly. In cases in which several calculated values of P_F were available, the value selected was that which made the experimental points for Na through Cs form the smoothest curve. The two forms of the screened interaction gave identical susceptibilities in the small Q limit within the numerical accuracy of the calculations. These calculated values are given in Table II for the metallic density range, and the Knight-shift data used and susceptibilities obtained from (50) are given in Table III.

The results of Silverstein[15] and those of Shimizu[14] were expressed in terms of χ/χ_P and plotted as a function of a_0k_F. Qualitatively these functions were quite similar to Pines', Silverstein's lying somewhat below and Shimizu's somewhat above on a plot similar to Fig. 12. Only Pines' was shown for clarity, and because it is representative. These results all show a slope in the metallic density region opposite to that of the present calculation and of the experimental results for Na, K, Rb, and Cs. Li gives a susceptibility quite out of line with the other alkali metals, and undoubtedly band structure corrections are important in this case.

[32] T. Muto, S. Kobayasi, and H. Kozima, J. Phys. Chem. Solids 23, 1303 (1962).

7. CONCLUSIONS

It is apparent from the results of Sec. 6 that, within the approximations used, the screening effect of the electron gas correlations renders the paramagnetic state stable relative to infinitesimal deformations. In fact, not even a remnant of the HF instability, which might have been expected to add structure to the $\chi(Q)$ curves, is evident. This result might have been anticipated from the study of the simplified interaction in Sec. 5, through which it became apparent that the antiferromagnetic instability was quite fragile, since any substantial reduction of the range of the interaction made the ferromagnetic instability dominant.

As noted previously, the absence of instabilities with respect to infinitesimal deformations does not establish the stability of the paramagnetic state. The HF SDW state should be used as a starting point for the calculation of the correlation energy to explore this point further.

The resemblance of the susceptibility functions obtained to that of the noninteracting gas indicates that the explanation of anomalously large oscillations in the indirect exchange interaction[6,7] should be sought elsewhere.[8]

The density dependence of the zero wave-vector susceptibility predicted by the present theory is in better qualitative agreement with experiment than that of previous theories. Although it is tempting to interpret such agreement as an indication that the reliability of the present calculation extends to lower electron densities than previous ones, the possible importance of band structure effects, which we have not included, leaves considerable doubt. We suggest that the low-density behavior we have calculated indicates the need for further investigation of the possibility of a ferromagnetic instability at lower density.

ACKNOWLEDGMENTS

One of the authors (D.R.H.) expresses his appreciation for the hospitality and support of the Ford Motor Company Scientific Laboratory during the performance of the major portion of this research. He thanks Professor G. W. Pratt for his aid and advice in supervising the thesis based on this research. The authors wish to thank Dr. A. D. Brailsford, Dr. N. Laurance, Dr. A. L. McWhorter, and Dr. R. Penny for many helpful discussions.

APPENDIX: GREEN'S FUNCTION DERIVATION OF THE SELF-ENERGY

The simplest screened interaction contribution to the dressed electron energy will be computed using the Green's function formalism. We will use the conventions of Abrikosov *et al.*,[33] and the reader is referred to their text for the development of the Green's function method.

In the particle-field formalism, the dressed Coulomb propagator is $v(\mathbf{q})/\epsilon(\mathbf{q},\omega)$, where ϵ is the dielectric function for causal boundary conditions. The bare one-electron Green's function is

$$G^0(\mathbf{k},\omega)=[\omega-\xi(\mathbf{k})+i\delta\,\mathrm{sgn}\xi(\mathbf{k})], \tag{A1}$$

where δ is a positive infinitesimal, sgn indicates "sign of," and

$$\xi(\mathbf{k})=\epsilon_{\mathbf{k}}-\epsilon_{k_F}. \tag{A2}$$

The simplest self-energy term, corresponding to the emission and reabsorption of one dressed field quantum, is

$$\Sigma(\mathbf{k},\omega)=i(2\pi)^{-4}\int d^3q\,d\omega' G^0(\mathbf{k}-\mathbf{q},\omega-\omega')v(\mathbf{q})/\epsilon(\mathbf{q},\omega'). \tag{A3}$$

In the nonrelativistic approximation we are using, the Coulomb propagator does not have the proper form for a true boson propagator, since $\epsilon(q,\omega)$ approaches unity as ω approaches infinity. Therefore we must make the decomposition

$$v(\mathbf{q})/\epsilon(\mathbf{q},\omega)=v(\mathbf{q})+D(\mathbf{q},\omega), \tag{A4}$$

where $D(\mathbf{q},\omega)$ approaches zero as ω approaches infinity, and thus possesses a Lehmann spectral representation,

$$D(\mathbf{q},\omega)=\int_0^\infty dt\mathfrak{D}(\mathbf{q},t)[(\omega-t+i\delta)^{-1}-(\omega+t-i\delta)^{-1}]. \tag{A5}$$

Substituing (A5) into (A4), we break Σ into two terms,

$$\Sigma(\mathbf{k},\omega)=\Sigma^{(1)}(\mathbf{k},\omega)+\Sigma^{(2)}(\mathbf{k},\omega), \tag{A6}$$

where

$$\Sigma^{(1)}(\mathbf{k},\omega)=i(2\pi)^{-4}\int d^3q d\omega' v(q)[\omega-\omega'-\xi(\mathbf{k}-\mathbf{q})+i\delta\,\mathrm{sgn}\xi(\mathbf{k}-\mathbf{q})]^{-1}. \tag{A7}$$

In cases such as (A7) where the contribution to the ω' integration from the circle at infinity does not vanish, we know from causality that the contour should be closed in the lower half ω' plane. The pole is only within the contour when $|\mathbf{k}-\mathbf{q}|<k_F$, so

$$\Sigma^{(1)}(\mathbf{k},\omega)=-(2\pi)^{-3}\int d^3q\,v(q)n_{\mathbf{k}-\mathbf{q}}, \tag{A8}$$

which is the ordinary exchange energy, as might have been anticipated.

[33] A. Abrikosov, L. Gorkov, and I. Dzyaloshinski, *Methods of Quantum Field Theory in Statistical Physics*, translated by R. Silverman (Prentice-Hall Inc., Englewood Cliffs, New Jersey, 1963).

The second contribution is

$$\Sigma^{(2)}(\mathbf{k},\omega)=\frac{i}{(2\pi)^4}\int d^3q \times d\omega' \frac{D(\mathbf{q},\omega')}{\omega-\omega'-\xi(\mathbf{k}-\mathbf{q})+i\delta\,\mathrm{sgn}\xi(\mathbf{k}-\mathbf{q})}$$
$$=\frac{i}{(2\pi)^4}\int d^3q\,d\omega'\left\{\frac{D(\mathbf{q},\omega')n_{\mathbf{k}-\mathbf{q}}}{\omega-\omega'-\xi(\mathbf{k}-\mathbf{q})-i\delta}+\frac{D(\mathbf{q},\omega')(1-n_{\mathbf{k}-\mathbf{q}})}{\omega-\omega'-\xi(\mathbf{k}-\mathbf{q})+i\delta}\right\}, \quad \text{(A9)}$$

where we have divided the $\mathbf{q}$ integration into two regions so that the pole of G° is above the real axis in one and below in the other. Substituting the spectral representation (A5) in (A9), we may interchange the orders of the integrations over t and ω'. The ω' contour may be closed in either half plane, since the contribution from infinity vanishes. Two of the four terms resulting from the substitution give zero because both poles are on the same side of the real axis. The remaining terms are

$$\Sigma^{(2)}(\mathbf{k},\omega)=\frac{i}{(2\pi)^4}\int d^3q(1-n_{\mathbf{k}-\mathbf{q}})\int_0^\infty dt\,\mathfrak{D}(\mathbf{q},t)\int_{-\infty}^\infty d\omega' \times\frac{1}{[\omega-\omega'-\xi(\mathbf{k}-\mathbf{q})+i\delta][\omega'-t+i\delta]}-\frac{i}{(2\pi)^4}$$
$$\times\int d^3q\,n_{\mathbf{k}-\mathbf{q}}\int_0^\infty dt\,\mathfrak{D}(\mathbf{q},t)\int_{-\infty}^\infty d\omega' \times\frac{1}{[\omega-\omega'-\xi(\mathbf{k}-\mathbf{q})-i\delta][\omega'+t-i\delta]}. \quad \text{(A10)}$$

The ω' integrations are simply done by residues, and after regrouping terms, we find

$$\Sigma^{(2)}(\mathbf{k},\omega)=-(2\pi)^{-3}\int d^3q\,n_{\mathbf{k}-\mathbf{q}}D(\mathbf{q},\omega-\xi(\mathbf{k}-\mathbf{q}))$$
$$+(2\pi)^{-3}\int d^3q\int_0^\infty dt\,\mathfrak{D}(\mathbf{q},t)[\omega-t-\xi(\mathbf{k}-\mathbf{q})+i\delta]^{-1}. \quad \text{(A11)}$$

We note from (A4) and (A5) that

$$\mathfrak{D}(\mathbf{q},t)=\pi^{-1}v(\mathbf{q})\,\mathrm{Im}\epsilon^{-1}(\mathbf{q},\omega). \quad \text{(A12)}$$

Combining (A11) and (A8), we obtain for the self-energy

$$\Sigma(\mathbf{k},\omega)=-(2\pi)^{-3}\int d^3q\,n_{\mathbf{k}-\mathbf{q}}v(q)\epsilon^{-1}(q,\omega-\xi(\mathbf{k}-\mathbf{q}))$$
$$-2^{-3}\pi^{-4}\int d^3q\,v(q)\int_0^\infty dt[\mathrm{Im}\epsilon^{-1}(q,t)] \times(\omega-t-\xi(\mathbf{k}-\mathbf{q})+i\delta)^{-1}. \quad \text{(A13)}$$

The dressed-electron Green's function is

$$G(\mathbf{k},\omega)=[\omega-\xi(\mathbf{k})-\Sigma(\mathbf{k},\omega)]^{-1}. \quad \text{(A14)}$$

The energy of the approximately stationary dressed electron state is taken to be the value of $\mathrm{Re}\omega$ at the pole of the analytic continuation of $G(\mathbf{k},\omega)$ nearest the real axis. To a first approximation, this is found by equating the real part of the denominator of (A14) to zero, substituting the bare electron energy in Σ.

$$E_k\approx\epsilon_k+\mathrm{Re}\Sigma[k,\xi(k)], \quad \text{(A15)}$$

where E_k is the dressed particle energy. Substituting our result (A13) for Σ gives

$$E_{\mathbf{k}}=\epsilon_{\mathbf{k}}-(2\pi)^{-3}\int d^3q\,n_{\mathbf{k}-\mathbf{q}}v(q)\,\mathrm{Re}\epsilon^{-1}(q,\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{k}-\mathbf{q}})$$
$$+2^{-3}\pi^{-4}\int d^3q\,v(q)P\int_0^\infty dt|\,\mathrm{Im}\epsilon^{-1}(q,t)| \times(\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{k}-\mathbf{q}}-t)^{-1}. \quad \text{(A16)}$$

Comparison with (23) shows that this is the same result obtained in Sec. 3.

This derivation is identical to that given by Quinn and Ferrell,[26] as may be seen by comparing their Eqs. (28) and (31) to our (A8) and (A9), with the substitution $\omega=\xi(\mathbf{k})$ already made in our equations. We have achieved a simplification in the handling of the contour integrals by our use of a spectral representation, and have cast our result in a different form from theirs to allow comparison with that of Sec. 3.