Plasmon-pole and paramagnon-pole model of an electron liquid

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The excitation spectrum of an electron liquid is represented by a simple, physically motivated model: Spin-symmetric excitations are replaced by a plasmon-pole spectrum, $\omega^{\rm pl}(q)$, and spin-antisymmetric excitations are replaced by a paramagnon-pole spectrum, $\omega^{\rm pa}(q)$. These frequencies are determined by requiring the model to have the correct density and spin response. Interaction of charged particles with plasmons and paramagnons is found by imposing the f-sum rules. With this model one can easily calculate both charge-induced and spin-induced correlation effects of interacting electrons. In one application we show that the model accounts for the significant narrowing of the occupied conduction band observed in several metals.

I. INTRODUCTION

An electron liquid with a uniform neutralizing background is still not fully understood from a microscopic point of view after nearly fifty years of intensive theoretical study.[1] At high densities there is a small perturbation parameter r_s, the equivalent sphere radius in Bohr units, which quantifies the strength of electron-electron interactions relative to the kinetic energy. When $r_s \ll 1$, standard perturbation analysis formulated in terms of Green's functions and diagrammatic expansions can be used. However, at metallic densities $2 < r_s < 6$ the "high-order" terms are as important as "low-order" terms. One has no right to keep only certain diagrams and neglect others. For metallic density one needs a simple, physically transparent, and motivated method to handle the correlation effects of interacting electrons.

Correlations are defined as the dynamical effects of the Coulomb interaction not included in a mean-field, Hartree-Fock (HF) Hamiltonian,

$$H_c = H - H_{\rm HF} \ . \tag{1}$$

These effects arise from both density fluctuations and spin fluctuations about the HF mean. A key problem is to find a simple way to deal with the complicated excitation spectrum of the electron liquid.

For a given wave-vector transfer $\mathbf{q}$ there are three types of excitation: electron-hole pairs, multipairs, and collective excitations.[2] Single-pair excitations require a double sum over momentum space. For multipair excitations the situation is even worse; for any q, the spectral width is infinity. Fortunately, in many cases, multipair excitations are much weaker than the other two.[2]

Density fluctuations of the system are related to the spin-symmetric part of the excitation spectrum, whereas spin fluctuations are related to the spin-antisymmetric part. The spin-symmetric collective excitations are the well-known plasmons. For small q the plasmon mode exhausts the f-sum rule.[3] For very large q, however, the single-pair excitations dominate. Since in this limit the spectral width becomes small compared to $\hbar^2 q^2/2m$, it is reasonable to collapse the spectrum into a single mode with $\hbar\omega^{\rm pl}(q) \to \hbar^2 q^2/2m$. A plasmon-pole model[4,5] has been developed to replace this excitation spectrum by a single plasmon branch $\hbar\omega(q)$, which is accurate for both small q and large q. As shown in Ref. 5 (hereafter referred to as I), the plasmon pole $\omega^{\rm pl}(q)$ can be determined by requiring the model to have a correct dielectric response. Interaction of plasmons with charged particles is found by imposing the f-sum rule. Thus the model carries the same oscillator strength as the true electron liquid for each q. The model enables one to easily calculate charge-induced correlation effects of an electron liquid.[5]

However, the plasmon-pole model only recognizes the spin-symmetric part of the excitation spectrum; it leaves the spin-antisymmetric part untouched. An electron couples to both charge fluctuations and spin fluctuations. It is the purpose of the present paper to treat both in a unified way. The paramagnon-pole spectrum $\omega_q^{\rm pa}$, the spin-antisymmetric partner of the plasmon-pole spectrum $\omega_q^{\rm pl}$, is determined by requiring the model to reproduce the correct spin susceptibility. Similar to the plasmon pole, the paramagnon pole also exhausts an f-sum rule (in vector form). But unlike the plasmons (which are scalar bosons) the paramagnons are vector bosons.

The beauty of the model is its simplicity in form and its ability to reproduce accurately (at the outset) several important physical response functions. Nevertheless, its limitations must be kept in mind. The model will become inaccurate for calculations which depend critically on the spectral width of the excitations. We shall demonstrate this in Sec. VII when we calculate the paramagnon-induced correlation energy $E_c^{\rm pa}(k)$.

The organization of the paper is as follows. In Sec. II, we refine the original development of the plasmon-pole model (formulated in I) so that the paramagnon-pole contribution can be derived straightforwardly in Sec. III. In Sec. IV, we study the electron liquid systematically to find quasiparticle properties, the correlation Hamiltonian of the system, etc. In Sec. V, we discuss the dielectric function and spin susceptibility of the electron liquid. From their general behavior we derive explicit dispersion curves for plasmon and paramagnon excitations (Sec. VI). Numerical calculations of the one-electron energy $E(\mathbf{k})$ are

given in Sec. VII. Narrowing of the occupied bandwidth observed in several metals is then explained. Finally, in Sec. VIII, our conclusions are summarized. In an appendix we comment on the relationship of this development to prior work.

II. PLASMON POLE

We consider a system of N electrons with a uniform (and rigid) positive background. The spin-symmetric part of the excitation spectrum is associated with the density fluctuations of the system,

$$\rho_{\mathbf{q}}=\sum_{\mathbf{k},\sigma} c^{\dagger}_{\mathbf{k}+\mathbf{q},\sigma}c_{\mathbf{k},\sigma} , \tag{2}$$

the spatial Fourier transform of the electron density. $c^{\dagger}_{\mathbf{k},\sigma}$ and $c_{\mathbf{k},\sigma}$ are creation and annihilation operators for an electron with momentum $\hbar\mathbf{k}$ and spin σ. The fundamental simplification of the model[5] is the representation of these fluctuations by plasmon creation and annihilation operators $a^{\dagger}_{\mathbf{q}}$ and $a_{\mathbf{q}}$ only:

$$\rho_{\mathbf{q}}=\Omega\lambda_q(a^{\dagger}_{\mathbf{q}}+a_{-\mathbf{q}}) , \tag{3}$$

where Ω is the total volume of the system.

As in I the coefficients λ_q are determined from the requirement that the model satisfy the f-sum rule. The f-sum rule is derived by evaluating the double commutator $[[H,\rho_{\mathbf{q}}],\rho^{\dagger}_{\mathbf{q}}]$. One obtains[6]

$$\sum_n \hbar\omega_{n0}\,|\,(\rho_{\mathbf{q}})_{n0}\,|^2=N\hbar^2q^2/2m . \tag{4}$$

$\hbar\omega_{n0}$ is the energy difference between the exact excited state n and the ground state. Since the plasmon-pole model assumes only one excitable density mode for each $\mathbf{q}$, Eq. (4) reduces to

$$\hbar\omega^{\mathrm{pl}}_q\Omega^2\lambda^2_q=N\hbar^2q^2/2m . \tag{5}$$

Thus the condition

$$\lambda_q=\left[\frac{q^2}{4\pi e^2}\,\frac{\hbar\omega_p^2}{2\Omega\omega^{\mathrm{pl}}_q}\right]^{1/2} \tag{6}$$

guarantees that the model carries the total oscillator strength. Here we have introduced the classical plasma frequency ω_p,

$$\omega_p=(4\pi Ne^2/m\Omega)^{1/2} . \tag{7}$$

The plasmon pole ω^{pl}_q, which incorporates all the oscillator strength, should approach ω_p as $q\to 0$ and $\hbar q^2/2m$ as $q\to\infty$. We will see that such behavior is a natural outcome of the following derivation.

In the linear-response regime an external field can probe the internal fluctuations. We apply a sinusoidal, static potential field $\phi(\mathbf{q})$ to the system in order to locate the plasmon pole ω^{pl}_q. Since the potential field only couples to the density fluctuations, the relevant interaction Hamiltonian is

$$H=H^{\mathrm{pl}}_{\mathrm{self}}-\frac{1}{\Omega}e\rho_{-\mathbf{q}}\phi(\mathbf{q}) . \tag{8}$$

The plasmon-pole model enables us to write down explicitly

$$H=\sum_{\mathbf{q}'}\hbar\omega^{\mathrm{pl}}_{\mathbf{q}'}a^{\dagger}_{\mathbf{q}'}a_{\mathbf{q}'}-e\lambda_q(a^{\dagger}_{-\mathbf{q}}+a_{\mathbf{q}})\phi(\mathbf{q}) . \tag{9}$$

The Hamiltonian given by (9) has the familiar harmonic oscillator form. It is straightforward, then, to evaluate the expectation values of the plasmon operators by the usual displacement trick

$$a^{\dagger}_{\mathbf{q}}\to a^{\dagger}_{\mathbf{q}}-\frac{e\lambda_q}{\hbar\omega^{\mathrm{pl}}_q}\phi(\mathbf{q}) . \tag{10}$$

Thereby we have

$$\langle a^{\dagger}_{\mathbf{q}}\rangle=\frac{e\lambda_q}{\hbar\omega^{\mathrm{pl}}_q}\phi(\mathbf{q}) .$$

Similarly,

$$\langle a_{\mathbf{q}}\rangle=\frac{e\lambda_q}{\hbar\omega^{\mathrm{pl}}_q}\phi(-\mathbf{q}) .$$

Using Eq. (3), we find the induced density

$$\langle\rho_{\mathbf{q}}\rangle=\frac{2e\Omega\lambda_q^2}{\hbar\omega^{\mathrm{pl}}_q}\phi(\mathbf{q}) . \tag{11}$$

The induced density must coincide with that given in terms of the static dielectric function $\epsilon(\mathbf{q})$ by the relation[2]

$$\frac{1}{\epsilon(\mathbf{q})}-1=-\frac{4\pi e\langle\rho_{\mathbf{q}}\rangle}{q^2\phi(\mathbf{q})} . \tag{12}$$

Inserting Eq. (11) into Eq. (12) and using Eq. (6) for λ_q, we obtain the plasmon frequency

$$\omega^{\mathrm{pl}}_q=\omega_p\left[\frac{\epsilon(q)}{\epsilon(q)-1}\right]^{1/2} . \tag{13}$$

This expression was derived in I by an electrostatic energy argument, but the present derivation is more easily applicable to spin fluctuations.

Once the static dielectric function $\epsilon(q)$ is given, Eq. (13) leads to a unique ω^{pl}_q which indeed has the desired limiting behaviors. It can be easily verified from well-known expressions for $\epsilon(q)$.[6]

In the plasmon-pole language, the interaction Hamiltonian between a test charge (at $\mathbf{r}$) and the plasmon modes is of the form

$$H_{t\text{-pl}}(\mathbf{r})=\sum_{\mathbf{q}}M^{\mathrm{pl}}_q(a^{\dagger}_{\mathbf{q}}e^{i\mathbf{q}\cdot\mathbf{r}}+a_{\mathbf{q}}e^{-i\mathbf{q}\cdot\mathbf{r}}) . \tag{14}$$

The coefficient M^{pl}_q is determined by a simple application of Poisson's equation; it is found that

$$M^{\mathrm{pl}}_q=\frac{4\pi e^2}{q^2}\lambda_q=\left[\frac{2\pi e^2\hbar\omega_p^2}{q^2\Omega\omega^{\mathrm{pl}}_q}\right]^{1/2} . \tag{15}$$

III. PARAMAGNON POLE

The spin-antisymmetric part of the excitation spectrum is associated with the spin fluctuations of the electron liquid,

$$S^{\nu}_{\mathbf{q}}=\sum_{\mathbf{k},\alpha,\beta} c^{\dagger}_{\mathbf{k}+\mathbf{q},\alpha}\sigma^{\nu}_{\alpha\beta}c_{\mathbf{k},\beta} , \tag{16}$$

the spectral Fourier transform of the spin density. σ^ν is the Pauli matrix in the νth direction. We may see immediately the essential difference between a spin fluctuation and a density fluctuation: A spin fluctuation has a vector character. The collective spin excitations, called paramagnons, are *vector* bosons.

It is easy to verify that spin fluctuations satisfy a vector f-sum rule,

$$\sum_n \hbar\omega_{n0}(S_{\mathbf{q}}^\nu)_{0n}(S_{\mathbf{q}}^{\mu\dagger})_{n0}=\left[\frac{N\hbar^2q^2}{2m}\right]\delta_{\nu\mu}\ . \tag{17}$$

$\hbar\omega_{n0}$, as before, is the energy difference between the exact excited state n and the ground state. The Pauli matrix identity,

$$(\sigma^\nu\sigma^\mu+\sigma^\mu\sigma^\nu)/2=\delta_{\nu\mu}\ , \tag{18}$$

has been used in obtaining Eq. (17).

Inspired by the success and advantages of the plasmon-pole model, we replace the entire spin-antisymmetric excitation spectrum by a single paramagnon mode $\omega_q^{\rm pa}$. (Since our system is isotropic, the frequency of the spin excitation $\omega_q^{\rm pa}$ is independent of the direction of $\mathbf{q}$.) Spin fluctuations are to be related to the paramagnon creation and annihilation operators,

$$S_{\mathbf{q}}^\nu=\Omega\eta_q(b_{\mathbf{q}\nu}^\dagger+b_{-\mathbf{q}\nu})\ . \tag{19}$$

The coefficient η_q is determined below.

In introducing the paramagnon creation and annihilation operators $b_{\mathbf{q}\nu}^\dagger$ and $b_{\mathbf{q}\nu}$ we should be aware of the noncommutativity of the spin components

$$[S_{\mathbf{q}}^\nu,S_{\mathbf{q}'}^\mu]=2i\epsilon_{\nu\mu\omega}S_{\mathbf{q}+\mathbf{q}'}^\omega\ . \tag{20}$$

Accordingly, the three paramagnon modes are not exactly independent of each other. However, this is not a serious difficulty. By using Eqs. (19) and (20), we have for $\nu\neq\mu$

$$[b_{\mathbf{q}\nu},b_{\mathbf{q},\mu}^\dagger]=O(1/\Omega)\ . \tag{21}$$

The noncommutativity is infinitesimal. This is a kinematic effect, and may be interpretd as a collision cross section between paramagnons. (A similar phenomenon occurs for magnons in ferromagnets.)

Accordingly the commutation relations for paramagnons are

$$\begin{aligned}&[b_{\mathbf{q}\nu},b_{\mathbf{q}'\mu}^\dagger]=\delta_{\mathbf{q}\mathbf{q}'}\delta_{\nu\mu}\ ,\\ &[b_{\mathbf{q}\nu},b_{\mathbf{q}'\mu}]=[b_{\mathbf{q}\nu}^\dagger,b_{\mathbf{q}'\mu}^\dagger]=0\ .\end{aligned} \tag{22}$$

From Eq. (19) the matrix element $(S_{\mathbf{q}}^\nu)_{n0}$ is zero unless the excited state n has a $\mathbf{q}$ paramagnon. Equation (17) then reduces to

$$\hbar\omega_q^{\rm pa}\Omega^2\eta_q^2=\frac{N\hbar^2q^2}{2m}\ . \tag{23}$$

In this way, the coefficient η_q (which determines the coupling strength of a paramagnon to an external probe) is obtained:

$$\eta_q=\left[\frac{N\hbar^2q^2}{2m\Omega^2\hbar\omega_q^{\rm pa}}\right]^{1/2}\ . \tag{24}$$

The paramagnon frequency $\omega_q^{\rm pa}$ is chosen so that the model reproduces the "correct" spin susceptibility. Consider a sinusoidal, static, magnetic field $B(\mathbf{q})$ applied to the system. Without loss of generality we take the field in the z direction. The Hamiltonian is then

$$H=H_{\rm self}^{\rm pa}+\frac{1}{\Omega}\mu_BS_{-\mathbf{q}}^zB(\mathbf{q})\ , \tag{25}$$

or

$$H=\sum_{\mathbf{q}',\nu}\hbar\omega_{q'}^{\rm pa}b_{\mathbf{q}'\nu}^\dagger b_{\mathbf{q}'\nu}+\mu_B\eta_q(b_{-\mathbf{q}z}^\dagger+b_{\mathbf{q}z})B(\mathbf{q})\ . \tag{26}$$

(μ_B is the Bohr magneton.)

By following a procedure similar to that from Eqs. (10)–(11), we obtain the expectation value of the induced spin fluctuation:

$$\langle S_{\mathbf{q}}^z\rangle=-\frac{2\mu_B\Omega\eta_q^2}{\hbar\omega_q^{\rm pa}}B(\mathbf{q})\ . \tag{27}$$

From the definition of the spin susceptibility

$$\chi_{\nu\mu}(\mathbf{q})=-\frac{\mu_B\langle S_{\mathbf{q}}^\nu\rangle}{B_\mu(\mathbf{q})}$$

the relation needed to define the paramagnon spectrum is found:

$$\frac{2\mu_B^2\Omega\eta_q^2}{\hbar\omega_q^{\rm pa}}=\chi(\mathbf{q})\ . \tag{28}$$

We assume, of course, that the spin susceptibility $\chi(\mathbf{q})$ is known. On replacing η_q in the above formula by the expression given in Eq. (24), we obtain finally

$$\omega_q^{\rm pa}=\left[\frac{N\mu_B^2q^2}{\Omega m\chi(\mathbf{q})}\right]^{1/2}\ . \tag{29}$$

We illustrate the application of the paramagnon-pole model by considering the effective interaction between two nuclear spins imbedded in an electron liquid at $\mathbf{r}_1$ and $\mathbf{r}_2$. The nuclear spins interact with the electron spins by the conventional Fermi contact interaction:

$$\begin{aligned}H(\mathbf{r}_1,\mathbf{r}_2)=&\frac{8\pi}{3}\hbar\gamma_1\mathbf{I}_1\cdot\mu_B\mathbf{S}(\mathbf{r}_1)\\ &+\frac{8\pi}{3}\hbar\gamma_2\mathbf{I}_2\cdot\mu_B\mathbf{S}(\mathbf{r}_2)\ .\end{aligned} \tag{30}$$

Here we employ the usual notation: $\hbar\gamma_i\mathbf{I}_i$ is the ith nuclear magnetic moment, and $\mathbf{S}(\mathbf{r}_i)$ is the spin density of the electron at $\mathbf{r}_i$.

With the help of Eq. (19) the interaction Hamiltonian can be rewritten as

$$H(\mathbf{r}_1,\mathbf{r}_2)=\sum_{\mathbf{q},\nu}\frac{8\pi}{3}\hbar\gamma_1\mu_B\eta_q(\mathbf{I}_i)_\nu(b_{\mathbf{q}\nu}e^{i\mathbf{q}\cdot\mathbf{r}_1}+b_{\mathbf{q}\nu}^\dagger e^{-i\mathbf{q}\cdot\mathbf{r}_1})+\sum_{\mathbf{q},\nu}\frac{8\pi}{3}\hbar\gamma_2\mu_B\eta_q(\mathbf{I}_2)_\nu(b_{\mathbf{q}\nu}e^{i\mathbf{q}\cdot\mathbf{r}_2}+b_{\mathbf{q}\nu}^\dagger e^{-i\mathbf{q}\cdot\mathbf{r}_2})\ . \tag{31}$$

In a manner similar to that of the phonon-mediated, electron-electron interaction in superconductivity, we obtain an indirect $\mathbf{I}_1\cdot\mathbf{I}_2$ interaction, involving virtual emission and absorption of paramagnons by the two nuclear spins. Since the splittings of the nuclear-spin levels are negligible, i.e., the off-shell energy transfer in the interaction is zero, we have accordingly

$$H_{\text{eff}}(\mathbf{r}_1,\mathbf{r}_2)=\sum_{\mathbf{q},\nu}\frac{2\Omega\left[\frac{8\pi}{3}\hbar\mu_B\eta_q\right]^2\gamma_1\gamma_2(\mathbf{I}_1)_\nu(\mathbf{I}_2)_\nu}{-\hbar\omega_q^{\text{pa}}}e^{i\mathbf{q}\cdot(\mathbf{r}_2-\mathbf{r}_1)}. \tag{32}$$

Using Eq. (28), we obtain

$$H_{\text{eff}}(\mathbf{r}_1,\mathbf{r}_2)=-\sum_{\mathbf{q}}\left[\frac{8\pi}{3}\hbar\right]^2\gamma_1\gamma_2\mathbf{I}_1\cdot\mathbf{I}_2\chi(\mathbf{q})e^{i\mathbf{q}\cdot(\mathbf{r}_2-\mathbf{r}_1)}, \tag{33}$$

which is a generalized Ruderman-Kittel (RK) interaction. If we use the noninteracting, electron-gas spin susceptibility $\chi^0(q)$ instead of $\chi(q)$, then $H_{\text{eff}}(\mathbf{r}_1,\mathbf{r}_2)$ is just the ordinary RK interaction.[7] A discussion of many-body corrections to the electron-liquid spin susceptibility (and consequently to the RK interaction) will be given in Sec. V.

IV. CORRELATION HAMILTONIAN

So far we have studied density and spin fluctuations of the electron liquid, and have described them by plasmons and paramagnons, respectively. We have also discussed the effects of such response on imbedded test charges or nuclear spins. However, we must now investigate the influence of plasmons and paramagnons on electrons themselves.

Consider one particular electron. The $N-1$ other electrons are to be regarded as a passive electron liquid and treated in the plasmon-pole and paramagnon-pole approximations. However, great care must be taken. Unlike a test charge, the electron creates an exchange hole, which modifies its coupling to the plasmons and paramagnons. The interaction can be evaluated in the following self-consistent way. Suppose the liquid has a density fluctuation for up-spin electrons, $\Delta n_\uparrow\cos(\mathbf{q}\cdot\mathbf{r})$, and $\Delta n_\downarrow\cos(\mathbf{q}\cdot\mathbf{r})$ for down-spin electrons. A probe electron, with momentum $\mathbf{k}$ and spin up, will experience a self-consistent potential $\phi_{\mathbf{k}\uparrow}(q)\cos(\mathbf{q}\cdot\mathbf{r})$. This potential will perturb the wave function of the electron:

$$\Psi_{\mathbf{k}\uparrow}=e^{i\mathbf{k}\cdot\mathbf{r}}+\alpha_{\mathbf{k}\uparrow}^{+}e^{i(\mathbf{k}+\mathbf{q})\cdot\mathbf{r}}+\alpha_{\mathbf{k}\uparrow}^{-}e^{i(\mathbf{k}-\mathbf{q})\cdot\mathbf{r}}. \tag{34}$$

This wave function has a periodically modulated charge density,

$$|\Psi_{\mathbf{k}\uparrow}|^2\cong 1+2(\alpha_{\mathbf{k}\uparrow}^{+}+\alpha_{\mathbf{k}\uparrow}^{-})\cos(\mathbf{q}\cdot\mathbf{r}). \tag{35}$$

Since each electron of the liquid can be considered as a probe electron, in turn, the perturbation coefficients $\alpha_{\mathbf{k}\uparrow}^{+}$, etc. must satisfy

$$\frac{2}{\Omega}\sum_{\mathbf{k}}(\alpha_{\mathbf{k}\uparrow}^{+}+\alpha_{\mathbf{k}\uparrow}^{-})=\Delta n_\uparrow(q). \tag{36}$$

There is a similar condition for down-spin electrons. Formally, Eq. (36) is an integral equation which cannot be solved until $\phi_{\mathbf{k}\uparrow}$ is related to $\Delta n_\uparrow$ (and $\Delta n_\downarrow$).

The self-consistent potential $\phi_{\mathbf{k}\uparrow}(q)$ is composed of a Hartree potential, an exchange potential, and a correlation potential:

$$\begin{aligned}\phi_{\mathbf{k}\uparrow}(q)=&V(q)[\Delta n_\uparrow(q)+\Delta n_\downarrow(q)]-2G_x(q)V(q)\Delta n_\uparrow(q)\\&-2G_c^p(q)V(q)\Delta n_\uparrow(q)\\&-2G_c^a(q)V(q)\Delta n_\downarrow(q),\end{aligned} \tag{37}$$

where $V(q)\equiv 4\pi e^2/q^2$. The corresponding equation for the down-spin potential is

$$\begin{aligned}\phi_{\mathbf{k}\downarrow}(q)=&V(q)[\Delta n_\uparrow(q)+\Delta n_\downarrow(q)]-2G_x(q)V(q)\Delta n_\downarrow(q)\\&-2G_c^p(q)V(q)\Delta n_\downarrow(q)\\&-2G_c^a(q)V(q)\Delta n_\uparrow(q).\end{aligned} \tag{38}$$

We have followed Kukkonen and Overhauser[8] by introducing the function $G_x(q)$ for the exchange correction (in the usual local-field approximation). The function $G_c^p(q)$ is the correlation correction arising from the parallel-spin modulation, whereas G_c^a is that for antiparallel spin. These functions were discussed previously by the authors.[9,10]

From the definitions of the density fluctuation, Eq. (2), and the spin fluctuation, Eq. (16), we have

$$\rho_{\mathbf{q}}\equiv\Delta n_\uparrow(q)+\Delta n_\downarrow(q), \tag{39}$$

and

$$S_{\mathbf{q}}^z\equiv\Delta n_\uparrow(q)-\Delta n_\downarrow(q). \tag{40}$$

We now replace $\Delta n_\sigma(q)$ in Eqs. (37) and (38) by $\rho_{\mathbf{q}}$ and $S_{\mathbf{q}}^z$:

$$\phi_{\mathbf{k}\uparrow}(\mathbf{q})=V(q)[1-G_+(q)]\rho_{\mathbf{q}}-G_-(q)V(q)S_{\mathbf{q}}^z, \tag{41}$$

and

$$\phi_{\mathbf{k}\downarrow}(\mathbf{q})=V(q)[1-G_+(q)]\rho_{\mathbf{q}}+G_-(q)V(q)S_{\mathbf{q}}^z. \tag{42}$$

Note that in the above expressions the spin-symmetric function,

$$G_+(q)=G_x(q)+G_c^p(q)+G_c^a(q), \tag{43}$$

enters the coupling between an electron and a *density* fluctuation, whereas the spin-antisymmetric function,

$$G_-(q)=G_x(q)+G_c^p(q)-G_c^a(q), \tag{44}$$

enters the coupling of an electron to a *spin* fluctuation.

Equations (41) and (42) can be extended to an electron having an arbitrary direction of spin $\mathbf{s}$. The general result is

$$\phi_{\mathbf{ks}}(\mathbf{q})=V(q)[1-G_+(q)]\rho_{\mathbf{q}}-G_-(q)V(q)\mathbf{s}\cdot\mathbf{S}_{\mathbf{q}}. \tag{45}$$

This self-consistent potential is the basis from which we calculate all correlation effects between a probe electron and the electron liquid.

With the help of the self-consistent potential, Eq. (45), we can now write down the total correlation Hamiltonian H_c of the electron system, in terms of the plasmon and paramagnon excitations:

$$H_c=\sum_{\mathbf{q}}\hbar\omega_q^{\mathrm{pl}}a_{\mathbf{q}}^{\dagger}a_{\mathbf{q}}+\sum_{\mathbf{q},\nu}\hbar\omega_q^{\mathrm{pa}}b_{\mathbf{q}\nu}^{\dagger}b_{\mathbf{q}\nu}+\sum_{\mathbf{k},\alpha}\sum_{\mathbf{q}}M_q^{\mathrm{pl}}[1-G_+(q)](a_{\mathbf{q}}^{\dagger}c_{\mathbf{k}-\mathbf{q},\alpha}^{\dagger}c_{\mathbf{k},\alpha}+a_{\mathbf{q}}c_{\mathbf{k}+\mathbf{q},\alpha}^{\dagger}c_{\mathbf{k},\alpha})$$
$$-\sum_{\mathbf{k},\alpha,\beta}\sum_{\mathbf{q},\nu}M_q^{\mathrm{pa}}G_-(q)\sigma_{\alpha\beta}^{\nu}(b_{\mathbf{q}\nu}^{\dagger}c_{\mathbf{k}-\mathbf{q},\alpha}^{\dagger}c_{\mathbf{k},\beta}+b_{\mathbf{q}\nu}c_{\mathbf{k}+\mathbf{q},\alpha}^{\dagger}c_{\mathbf{k},\beta})\ . \tag{46}$$

ν is the index corresponding to the three components of the vector paramagnon. M_q^{pl} is given by Eq. (15). It is clear that, as pointed out in I, the electron couples to the density fluctuations with strength $M_q^{\mathrm{pl}}[1-G_+(q)]$.[11] From Eqs. (19), (24), and (46), we see that

$$M_q^{\mathrm{pa}}=V(q)\eta_q=\frac{4\pi e^2}{q^2}\left[\frac{N\hbar^2q^2}{2m\Omega^2\hbar\omega_q^{\mathrm{pa}}}\right]^{1/2}\ . \tag{47}$$

The electron couples to spin fluctuations through the many-body correction $G_-(q)$, i.e., with strength $M_q^{\mathrm{pa}}G_-(q)$.

The correlation Hamiltonian H_c provides all the information needed to study dynamic response of an electron liquid to a probe electron. The first two terms on the right-hand side of Eq. (46) are the excitation energies of plasmons and paramagnons. The third term leads to charge-induced correlations (through virtual emission and absorption of plasmons). The fourth term leads to spin-induced correlations. Note that the paramagnon-mediated interaction can cause electrons to flip their spins. From H_c we can easily derive the Kukkonen-Overhauser[8] (KO) electron-electron interaction. Specifically, the plasmon-mediated interaction, when added to the bare Coulomb interaction $4\pi e^2/q^2$, leads to the spin-symmetric part, and the paramagnon-mediated interaction yields the spin-antisymmetric part of the KO interaction.[10]

V. $G_+(q)$ AND $G_-(q)$

The formulas derived so far are in general form, since the relevant dielectric function $\epsilon(q)$ and spin susceptibility $\chi(q)$ are not specified. This is one advantage of our model. One is free to choose his own favorite $\epsilon(q)$ or $\chi(q)$.

The static dielectric function $\epsilon(q)$ and spin susceptibility $\chi(q)$ are usually written as

$$\epsilon(q)=1+\frac{Q(q)}{1-G_+(q)Q(q)} \tag{48}$$

and

$$\chi(q)=-\frac{\mu_B^2\Pi^0(q)}{1-G_-(q)Q(q)}\ . \tag{49}$$

We have used the notation $Q(q)=-V(q)\Pi^0(q)$, where $\Pi^0(q)$ stands for the Lindhard free-electron response function

$$\Pi^0(q)=-\frac{mk_F}{\pi^2\hbar^2}f(q/2k_F)\ , \tag{50}$$

with

$$f(x)=\frac{1}{2}+\frac{1-x^2}{4x}\ln\left|\frac{1+x}{1-x}\right|\ . \tag{51}$$

Unfortunately, the many-body corrections G_+ and G_- are still unknown after more than a quarter of a century of intensive research following the pioneering work of Hubbard.[12] We shall be content to use simple functions for G_+ and G_-, based on heuristic interpolation between known limits, in order to carry on with numerical calculations.

The strategy is based on knowledge of G_+ and G_- for small and large q. It is well known that the small-q behavior of the static dielectric function $\epsilon(q)$ is determined by the compressibility relation.[2] Since in this limit there exists a relation between the compressibility of the system κ and $\epsilon(q)$, as derived in I,

$$\kappa=\lim_{q\to0}\frac{q^2}{4\pi n^2e^2}\epsilon(q)\ , \tag{52}$$

where $n=N/\Omega$ is the electron density. This relation can be used to find the behavior of $G_+(q)$ as $q\to0$.

We know that the compressibility κ is related to the ground-state energy of the system W by

$$\frac{1}{\kappa}=\Omega\frac{\partial^2W}{\partial\Omega^2}\ . \tag{53}$$

On the other hand, the energy W of the electron liquid is

$$W=N[\tfrac{3}{5}(\hbar^2k_F^2/2m)-3e^2k_F/4\pi+w_c]\ . \tag{54}$$

The first two terms are the kinetic and exchange energies, and w_c is the correlation energy per electron. In the past 50 years there have been countless calculations of w_c for metallic densities.[1] All substantially agree with each other, and are also in a good agreement with recent Monte Carlo variational calculations.[13] Furthermore they lead to nearly correct cohesive energies for simple metals.[14] For $1\le r_s<6$, Singwi and Tosi[1] found an analytic expression,

$$w_c(r_s)=\left[-0.112+0.0335\ln r_s-\frac{0.02}{0.1+r_s}\right]\frac{me^4}{2\hbar^2}\ , \tag{55}$$

which is a very good representation of w_s in the region.

We now combine Eqs. (48), (52), (53), and (54), with Ω and k_F (expressed in terms of r_s), and obtain

$$\lim_{q\to0}\frac{G_+(q)}{x^2}\equiv1+\alpha\ , \tag{56}$$

with $x\equiv q/2k_F$ and

$$\alpha=\frac{2\pi}{3}\left[\frac{4}{9\pi}\right]^{1/3}(\hbar^2r_s^2/me^4)\left[\frac{dw_c}{dr_s}-\frac{r_s}{2}\frac{d^2w_c}{dr_s^2}\right]\ . \tag{57}$$

Inserting (55) into (57), we get

$$\alpha=\left[\frac{2\pi}{3}\right]^{2/3}r_s\left[\frac{0.0335}{2}+\frac{0.02r_s}{3(0.1+r_s)^2}\left[1+\frac{r_s}{0.1+r_s}\right]\right]\ . \tag{58}$$

Consider next the small-q behavior of $G_-(q)$. Hamann and Overhauser,[15] for example, have calculated the spin susceptibility $\chi(q)$, whose small-q value [on recalling the definition (49)] can be used to determine $G_-(q)$ in the limit $q\to 0$. Several experiments have attempted to measure $\chi(0)$ as the function of r_s.[16] The results substantially agree with the theoretical values.[15] Introducing the Pauli spin susceptibility, $\chi_p=-\mu_B^2\Pi^0(0)$, the zero-q susceptibility, $\chi(0)$, as a function of r_s can be reexpressed as

$$\chi(0)/\chi_p=1.17+0.029(r_s-1)^2+0.175\ln r_s\ . \tag{59}$$

With the help of Eqs. (49)—(51), we get

$$\lim_{q\to 0} G_-(q)/x^2=\frac{1}{0.166r_s}\left[1-\frac{\chi_p}{\chi(0)}\right]\ . \tag{60}$$

In the opposite extreme the large-q behaviors of $G_+(q)$ and $G_-(q)$ have been studied by the equation-of-motion method. The method was first used by Niklasson[17] to study the density response of the electron liquid. He found an exact condition on $G_+(q)$:

$$\lim_{q\to\infty} G_+(q)=\tfrac{2}{3}[1-g(0)]\ , \tag{61}$$

where $g(r)$ is the pair correlation function. Recently, we obtained a corresponding result for $G_-(q)$ by studying the spin response of an electron liquid,[9]

$$\lim_{q\to\infty} G_-(q)=\tfrac{1}{3}[4g(0)-1]\ . \tag{62}$$

The value of the pair distribution function $g(\mathbf{r})$ at $r=0$ depends on r_s also. Overhauser derived an approximate formula.[18]

$$g(0)=\frac{32}{(8+3r_s)^2}\ , \tag{63}$$

which is in good agreement with recent calculations.[19]

It is surprising to note that, from Eqs. (62) and (63), at metallic densities the many-body correction $G_-(q)$ is negative for large q, opposite in sign to the limit at small q. So the spin susceptibility for large q is suppressed, rather than enhanced, by many-body effects.

With the help of the foregoing limits we can interpolate general expressions for $G_+(q)$ and $G_-(q)$. The usual (and simplest) way to interpolate $G_+(q)$ was first suggested by Hubbard:[12]

$$G_+(q)=\frac{(1+\alpha)x^2}{1+(1+\alpha)x^2/G_+(\infty)} \tag{64}$$

is a smooth function having the correct limiting values. The curves in Fig. 1 are for an electron liquid with the conduction-electron density of Na ($r_s=3.93$). However, there is a possibility that $G_+(q)$ has a peak near $q=2k_F$,[20] a residue of the enormous peak caused by exchange effects.[21] In Fig. 1 we also show a function $G'_+(q)$ with a Lorentzian peak added to Eq. (64), i.e.,

$$G'_+(q)=G_+(q)+\frac{P\Gamma^2x^2}{(1-x^2)^2+\Gamma^2}\ . \tag{65}$$

P is the height of the peak (at $x=1$) and Γ is its width.

Construction of a suitable $G_-(q)$ needs somewhat more consideration. Since $G_-(q)$ increases quadratically with q (for small q), but then approaches (asymptotically) a negative value, it is important to discover where the function has a maximum. We shall assume that the large exchange peak at $q=2k_F$ is not completely swamped by correlation effects, so we look for a simple function having a maximum near $2k_F$. An appropriate one is

$$G_-(q)=\frac{\beta x^2+\gamma x^4}{1+[\gamma x^4/G_-(\infty)]}\ . \tag{66}$$

β is defined to be the right-hand side of Eq. (60). γ is chosen so that the maximum of $G_-(q)$ falls at $q=2k_F$, i.e., $x=1$. Accordingly,

$$\gamma\equiv\frac{\beta G_-(\infty)}{-2G_-(\infty)+\beta}\ . \tag{67}$$

$G_-(q)$ is also shown in Fig. 1. It has the correct behavior at $q=0$ and ∞, and has its maximum at $x\equiv q/2k_F=1$.

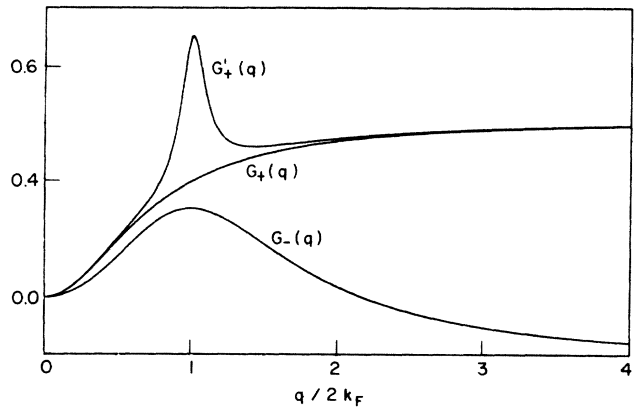

FIG. 1. Exchange and correlation local-field corrections, $G_+(q)$ and $G_-(q)$, for an electron liquid having the electron density of Na ($r_s=3.93$). Whether or not G_+ has a peak at $q=2k_F$, as shown by the curve G'_+, is an open question. See Ref. 20.

VI. DISPERSION CURVES FOR $\omega_q^{\rm pl}$ AND $\omega_q^{\rm pa}$

With definite expressions for $G_+(q)$ and $G_-(q)$, we are now able to specify dispersion curves for both the plasmon pole and paramagnon pole. The dielectric function, Eq. (48), and the dispersion relation, Eq. (13), can be combined to give

$$\omega_q^{\rm pl}=\omega_P\left[\frac{1+[1-G_+(q)]Q(q)}{Q(q)}\right]^{1/2}\ . \tag{68}$$

This function is shown in Fig. 2 for an electron density equal to that of Na. (For this density the classical plasmon frequency is $\hbar\omega_P=6.05$ eV.) The small-q behavior,

$$\hbar\omega_q^{\rm pl}=6.05+1.22x^2\ , \tag{69}$$

persists till $q\sim k_F$. In the transition regime $k_F<q<2k_F$ the plasmon dispersion flattens slightly as the plasmon pole incorporates the single electron-hole—pair excitation

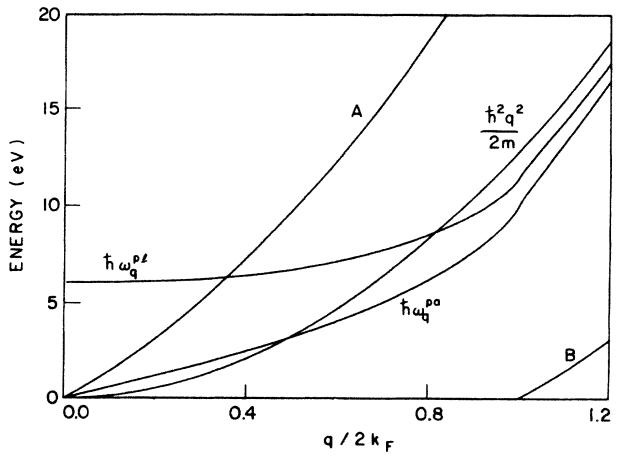

FIG. 2. Excitation spectrum (versus wave-vector transfer q) for an electron liquid with the density of Na. The free-electron spectrum is the entire region between curves A and B. In this paper all spin-symmetric excitations are collapsed into the plasmon-pole mode $\hbar\omega_q^{\rm pl}$, while all spin-antisymmetric excitations are collapsed into the paramagnon-pole mode $\hbar\omega_q^{\rm pa}$. Both modes approach $\hbar^2q^2/2m$ for $q \gg 2k_F$.

strength. For $q > 2k_F$ the single-pair excitations gradually dominate, so $\omega_q^{\rm pl}$ approaches the center of the continuum, $\omega = \hbar q^2/2m$. Experimentally such a plasmon dispersion spectrum was found in Al.[22]

The effect of a peak in $G_+(q)$ [see Eq. (65)] would be to bend the curve in a small region near $q \sim 2k_F$. It would flatten the curve even more for $q < 2k_F$ and would cause a steeper rise for $q > 2k_F$.

If one combines Eqs. (29) and (49), the dispersion relation for the paramagnon pole is found:

$$\omega_q^{\rm pa} = \left[\frac{1-G_-(q)Q(q)}{3f(x)}\right]^{1/2} v_F q \ , \tag{70}$$

where v_F is the Fermi velocity. If the many-body correction $G_-(q)$ were neglected, the paramagnon velocity would be $v_F/\sqrt{3}$ for small q. Our paramagnon pole near $q=0$ resembles the "paramagnetic spin wave" studied by Van Zandt,[23] who employed a time-dependent HF approximation. With $G_-(q)$ given by Eq. (66), the paramagnon dispersion spectrum was calculated. The result is shown in Fig. 2. For large-q this curve also approaches $\omega = \hbar q^2/2m$, as expected.

VII. CORRELATION ENERGY $E_c(\mathbf{k})$

Using the correlation Hamiltonian H_c, Eq. (46), one can calculate the $\mathbf{k}$-dependent correlation energy $E_c(\mathbf{k})$. In doing so, we first evaluate the total correlation energy of the system, which is given by second-order Brillouin-Wigner perturbation theory:[24]

$$W_c = \sum_{\mathbf{k}}\sum_{\mathbf{q}} \frac{(M_q^{\rm pl})^2[1-G_+(q)]^2}{E(\mathbf{k})-E(\mathbf{k}-\mathbf{q})-\hbar\omega_q^{\rm pl}} n_{\mathbf{k}}(1-n_{\mathbf{k}-\mathbf{q}}) + \sum_{\mathbf{k}}\sum_{\mathbf{q}} \frac{3[M_q^{\rm pa}G_-(q)]^2}{E(\mathbf{k})-E(\mathbf{k}-\mathbf{q})-\hbar\omega_q^{\rm pa}} n_{\mathbf{k}}(1-n_{\mathbf{k}-\mathbf{q}}) \ . \tag{71}$$

$n_{\mathbf{k}}$ is the ground-state occupation number. (The factor 3 in the last term arises from the vector character of the paramagnons.)

The $E(\mathbf{k})$ occurring in the denominators of Eq. (71) are the one-electron energies, and should be determined self-consistently:

$$E(k) = \frac{\partial}{\partial n_{\mathbf{k}}}(W_{\rm HF}+W_c) \ , \tag{72}$$

and is the sum of three contributions:

$$E(k) = \hbar^2k^2/2m + E_x(k) + E_c(k) \ . \tag{73}$$

The second term is the exchange energy

$$E_x(k) = -\frac{1}{\Omega}\sum_{k'<k_F} \frac{4\pi e^2}{|\mathbf{k}'-\mathbf{k}|^2} \ , \tag{74}$$

which can be readily evaluated. If we define $y \equiv k/k_F$,

$$E_x(k) = -(2e^2k_F/\pi)f(y) \ , \tag{75}$$

where $f(y)$ is the same function that appears in Eq. (51). Differentiation of Eq. (71) with respect to $n_{\mathbf{k}}$ gives the one-electron correlation energy $E_c(\mathbf{k})$,

$$\frac{\partial W_c}{\partial n_{\mathbf{k}}} = E_c(k) = E_c^{\rm pl}(k) + E_c^{\rm pa}(k) \ , \tag{76}$$

with

$$E_c^{\rm pl}(k) = \sum_{\mathbf{q}} (M_q^{\rm pl})^2[1-G_+(q)]^2 \left[\frac{1-n_{\mathbf{k}-\mathbf{q}}}{E(\mathbf{k})-E(\mathbf{k}-\mathbf{q})-\hbar\omega_q^{\rm pl}} - \frac{n_{\mathbf{k}+\mathbf{q}}}{E(\mathbf{k}+\mathbf{q})-E(\mathbf{k})-\hbar\omega_q^{\rm pl}}\right] \tag{77}$$

and

$$E_c^{\rm pa}(k) = \sum_{\mathbf{q}} 3[M_q^{\rm pa}G_-(q)]^2 \left[\frac{1-n_{\mathbf{k}-\mathbf{q}}}{E(\mathbf{k})-E(\mathbf{k}-\mathbf{q})-\hbar\omega_q^{\rm pa}} - \frac{n_{\mathbf{k}+\mathbf{q}}}{E(\mathbf{k}+\mathbf{q})-E(\mathbf{k})-\hbar\omega_q^{\rm pa}}\right] . \tag{78}$$

$E_c^{\rm pl}(k)$, given by Eq. (77), is the plasmon-induced correlation energy. Its first term is the second-order energy arising from the virtual emission and reabsorption of a plasmon $\mathbf{q}$. The electron at $\mathbf{k}$ is virtually excited to an empty state $\mathbf{k}'=\mathbf{k}-\mathbf{q}$ above the Fermi surface. The second term occurs when $\mathbf{k}$ is empty. The hole at $\mathbf{k}$ is virtually excited to filled states $\mathbf{k}+\mathbf{q}$ below the Fermi surface. Similar remarks apply to the paramagnon-induced correlation energy $E_c^{\rm pa}(k)$.

The k-dependent, plasmon-induced correlation energy $E_c^{\rm pl}(k)$, calculated for $r_s=3.93$, is shown in Fig. 3 and was taken from Ref. 5. $E_c^{\rm pl}(k)$ is relatively insensitive to

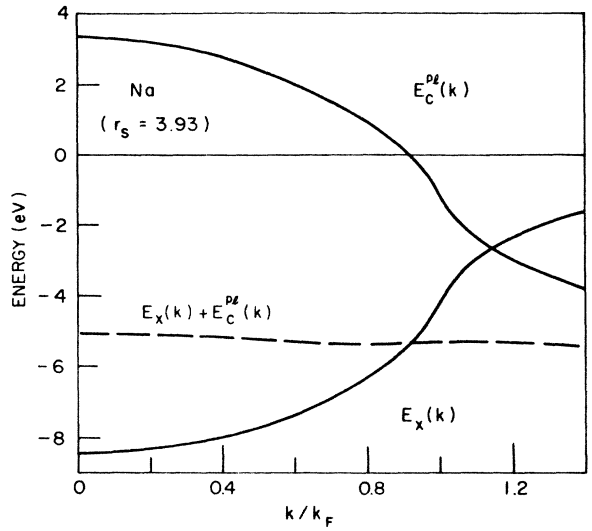

FIG. 3. Plasmon-induced correlation energy $E_c^{\rm pl}(k)$, exchange energy $E_x(k)$, and their sum. Both solid curves have logarithmically singular slopes at $k=k_F$, but the singularities cancel in the sum. (This figure is taken from Ref. 5.)

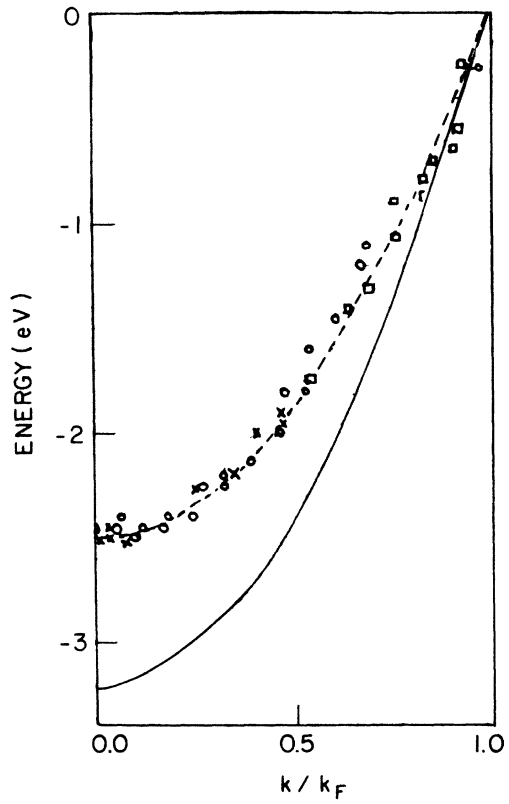

FIG. 4. Measured $E(k)$ for the Na conduction band. The solid curve is a free-electron spectrum, and the dashed curve is an effective-mass band with $\overline{m}=1.28m$. The Fermi energy is defined to be zero. Data are from Jensen and Plummer, Ref. 25.

the choice of $G_+(q)$. For example, the effect of the peak in $G'_+(q)$ is almost unnoticeable. It should be noted that for most $k<k_F$, $E_c^{\rm pl}$ is positive. This can be traced to the fact that virtual transitions to a small-k empty state are more effective than virtual transitions from a filled state. $E_c^{\rm pl}$ falls precipitously near k_F, and has a logarithmic singularity equal and opposite to a corresponding one in the exchange energy $E_x(k)$. Notice that the sum $E_x+E_c^{\rm pl}$ is almost independent of k for $k<1.4k_F$. This sum is shown by the dashed line in Fig. 3.

We now define a mean mass $\overline{m}$:

$$\hbar^2k_F^2/2\overline{m}\equiv E(k_F)-E(0)\ . \tag{79}$$

Were we to exclude the paramagnon contribution, this "bandwidth" mass for Na would be 1.055. This value corresponds to a 0.17-eV reduction from the free-electron bandwidth. The observed reduction, found recently by Jensen and Plummer[25] and shown in Fig. 4, is 0.7 eV. Thus the experimental mean mass is $\overline{m}/m=1.28$. This discrepancy can be accounted for by the paramagnon term in $E(k)$.

Angle-resolved photoemission (utilizing synchrotron radiation) has been used to measure the occupied and unoccupied band structure of several metals.[26,27] The large bandwidth narrowing found in Be and Al cannot be explained by the electron-plasmon interaction. For Na, where the periodic potential of the ion lattice has negligible effect, it seems evident that an improved many-body theory is required. We now show that the electron-paramagnon interaction, which has previously been neglected, explains the unexpectedly large $\overline{m}$'s.

Before one evaluates the paramagnon-induced correlation energy $E_c^{\rm pa}(k)$, it is worthwhile to examine the corresponding expression, Eq. (77), for $E_c^{\rm pl}(k)$. The minimum value of $\omega_q^{\rm pl}$ is the classical plasmon frequency ω_P, e.g., 6.05 eV for Na. Vanishing of the energy denominator,

$$E(\mathbf{k}_c)-E(\mathbf{k}_c-\mathbf{q}_c)-\hbar\omega_{q_c}^{\rm pl}=0\ , \tag{80}$$

in the integrand of Eq. (77) cannot occur until k reaches $k_c\sim 1.7k_F$. Therefore, as long as k is sufficiently small compared to k_c, the spectral width of the density excitations is unimportant, and the plasmon-pole model is reasonably accurate. (k_c is the threshold wave vector at which an electron can excite a real plasmon.) One expects an interesting feature to appear in $E_c^{\rm pl}(k)$ where $k\sim k_c$. Such an anomaly was first predicted by Hedin and Lundquist.[4] Because the energy denominator, Eq. (80), becomes small when this occurs, the finite width of the spectral density must be incorporated into the plasmon-pole approximation when $E_c^{\rm pl}(k)$ is computed for k near k_c. Observation of this plasmon anomaly has recently been reported by Jensen *et al.*[27]

It is clear from Fig. 2 that, unlike the plasmon spectrum $\omega_q^{\rm pl}$, the paramagnon branch $\omega_q^{\rm pa}$ is completely immersed in the single-particle excitation continuum. Accordingly, all paramagnon modes will suffer Landau damping. (Any paramagnon can always be annihilated by creation of an electron-hole pair.) Therefore, one must *not* evaluate $E_c^{\rm pa}(k)$ from Eq. (78), even for small k. In-

stead, the calculation must incorporate the finite spectral width of the spin excitations.

Accordingly we generalize Eq. (78) by introducing a Landau-damping spectral density $P(\omega)$ (Ref. 28) to replace the (infinitely sharp) paramagnon pole,

$$P(\omega)=\frac{2\omega^2\Gamma_q/\pi}{(\omega^2-\omega_q^{\mathrm{pa}2})^2+\omega^2\Gamma_q^2} . \tag{81}$$

The modified Eq. (78) is, then,

$$E_c^{\mathrm{pa}}(k)=3\sum_{\mathbf{q}}\int_0^\infty d\omega\, P(\omega)[M_q^{\mathrm{pa}}G_-(q)]^2\left[\frac{1-n_{\mathbf{k}-\mathbf{q}}}{E(\mathbf{k})-E(\mathbf{k}-\mathbf{q})-\hbar\omega}-\frac{n_{\mathbf{k}+\mathbf{q}}}{E(\mathbf{k}+\mathbf{q})-E(\mathbf{k})-\hbar\omega}\right] . \tag{82}$$

Following Danino and Overhauser,[28] we calculate the damping constant Γ_q by using standard transition-rate theory:

$$\Gamma_q=\sum_{\mathbf{k},\alpha,\beta}\frac{2\pi}{\hbar}\langle\mathbf{k}\pm\mathbf{q},\beta\,|\,H_{e\text{-pa}}\,|\,\mathbf{k},\alpha\rangle^2\rho(\omega_q^{\mathrm{pa}}) . \tag{83}$$

$H_{e\text{-pa}}$ is the electron-paramagnon interaction Hamiltonian, Eq. (46). For a given $\mathbf{q}$ and polarization ν, we have

$$H_{e\text{-pa}}=-\sum_{\mathbf{k},\alpha,\beta}M_q^{\mathrm{pa}}G_-(q)\sigma_{\alpha\beta}^{\nu}(b_{\mathbf{q}\nu}^{\dagger}c_{\mathbf{k}-\mathbf{q},\alpha}^{\dagger}c_{\mathbf{k},\beta}+b_{\mathbf{q}\nu}c_{\mathbf{k}+\mathbf{q},\alpha}^{\dagger}c_{\mathbf{k},\beta}) . \tag{84}$$

Equations (83) and (84), together with the Pauli matrix identity (18), lead to

$$\Gamma_q=\frac{2\pi}{\hbar}[M_q^{\mathrm{pa}}G_-(q)]^2\sum_{\mathbf{k},\alpha}\rho(\omega_q^{\mathrm{pa}}) . \tag{85}$$

The density of final states $\rho(\omega_q^{\mathrm{pa}})$ is that appropriate to the single-particle excitations having energy transfer ω_q^{pa} and momentum transfer $\mathbf{q}$. The summation in Eq. (85) was evaluated in Ref. 28:

$$\sum_{\mathbf{k},\alpha}\rho(\omega_q^{\mathrm{pa}})=\frac{m^2\omega_q^{\mathrm{pa}}}{\pi^2\hbar^3q} . \tag{86}$$

Equations (85) and (86) determine the paramagnon damping Γ_q.

Equation (82) can now be evaluated numerically. The result for Na ($r_s=3.93$) is shown in Fig. 5. It is apparent that the electron-paramagnon interaction significantly increases the mean mass $\overline{m}$, Eq. (79). It reduces the width of the conduction band by 0.66 eV. Since the observed reduction is about 0.7 eV,[25] we conclude that the electron-paramagnon interaction is the main cause of bandwidth narrowing in simple metals. Figure 6 is the one-electron energy $E(k)$ from Eq. (73). The curve has been adjusted so that it coincides with the free-electron curve at E_F. This theoretical $E(k)$ should be compared with the experimental one shown in Fig. 4.

Various energy and mass values are given in Table I for electron densities appropriate to seven "jellium" metals. Contributions from band structure and electron-phonon interactions have of course been omitted. Comparison of the fifth and seventh rows shows that the paramagnon contribution to the correlation energy is less than 10% of the sum of the exchange and plasmon contributions.

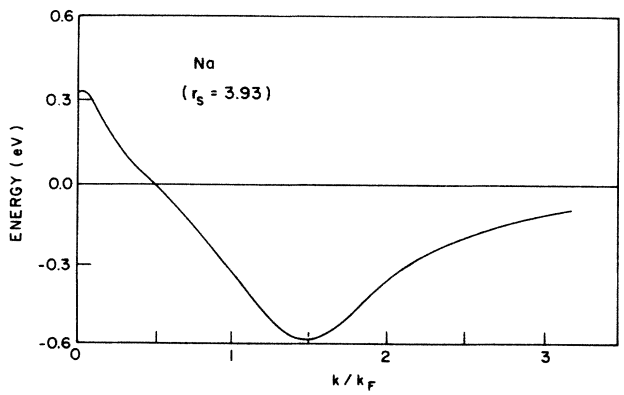

FIG. 5. Paramagnon-induced correlation energy $E_c^{\mathrm{pa}}(k)$.

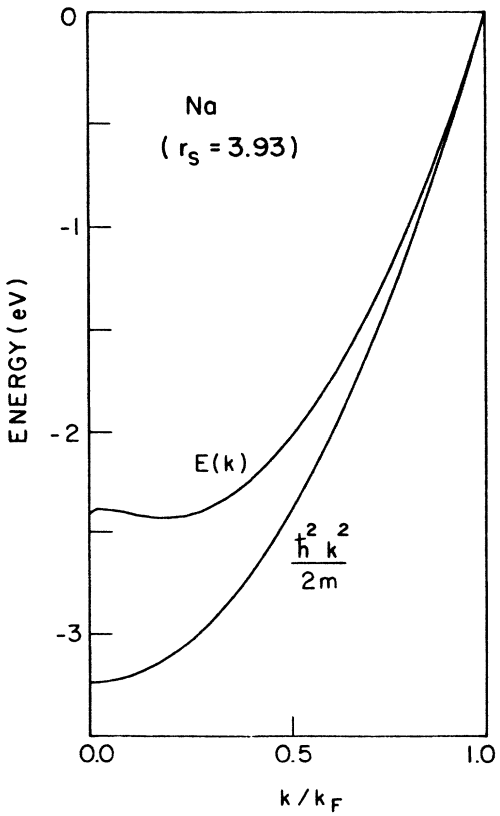

FIG. 6. Theoretical $E(k)$ for an electron (quasiparticle) which includes all the many-body effects presented in this paper. The free-electron parabola is shown for comparison.

TABLE I. Calculated energy and mass values for electron liquids having densities equal to those of seven "jellium" metals. Energies are in eV.

	Be	Al	Li	Na	K	Rb	Cs
r_s	1.88	2.07	3.25	3.93	4.87	5.12	5.62
$\hbar\omega_P$	18.28	15.78	8.05	6.05	4.39	3.98	3.53
$\hbar^2k_F^2/2m$	14.18	11.65	4.75	3.24	2.12	1.86	1.58
$E_c^{pa}(0)$	1.17	1.12	0.64	0.31	−0.03	−0.10	−0.19
$E_c^{pa}(k_F)$	−0.51	−0.48	−0.38	−0.35	−0.33	−0.32	−0.31
$E_x(0)+E_c^{pl}(0)$	−10.25	−9.32	−6.04	−5.05	−4.16	−3.97	−3.65
$E_x(k_F)+E_c^{pl}(k_F)$	−10.29	−9.41	−6.22	−5.22	−4.30	−4.11	−3.77
$\overline{m}/m$	1.137	1.171	1.337	1.344	1.260	1.231	1.170
m^*/m	0.974	0.979	1.023	1.067	1.140	1.166	1.225

VIII. CONCLUSIONS

We have shown that the plasmon-pole and paramagnon-pole model provides an easy method for calculating both charge-induced and spin-induced correlation effects of interacting electrons. With this model one can easily calculate the one-electron energy spectrum. Although the sum of $E_x(k)$ and $E_c^{pl}(k)$ makes a very small contribution to the mean mass $\overline{m}$, the paramagnon-induced correlation energy $E_c^{pa}(k)$ increases $\overline{m}$ by a significant amount. It explains the narrowing of the conduction-electron bandwidth observed in several metals. Damping of the paramagnon modes must be incorporated in situations where the finite spectral width is important.

ACKNOWLEDGMENT

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APPENDIX: COMPARISON WITH SEVERAL PREVIOUS MANY-BODY THEORIES

The essence of the model presented here is to replace density fluctuations of an electron liquid by a single plasmon mode (a scalar boson), and the spin fluctuations by a paramagnon mode (a vector boson). Consequently, the correlation Hamiltonian of the system is greatly simplified and becomes a tractable operator H_c. From H_c, Eq. (46), one can easily calculate several many-body effects.

In order to compare our work to previous many-body theories (formulated in terms of Green's functions and diagrammatic expansions) we introduce the free propagator

$$D^{pl}(\mathbf{q},\omega)=\frac{2\hbar\omega_q^{pl}}{(\hbar\omega)^2-(\hbar\omega_q^{pl})^2} \tag{A1}$$

for plasmons, and

$$D_\nu^{pa}(\mathbf{q},\omega)=\frac{2\hbar\omega_q^{pa}}{(\hbar\omega)^2-(\hbar\omega_q^{pa})^2} \tag{A2}$$

for paramagnons. Equation (77) for the plasmon-induced correlation energy $E_c^{pl}(k)$ is equivalent to the irreducible self-energy[2]

$$\Sigma_c^{pl}(\mathbf{k},k_0)=i\Omega\int\frac{d^3q}{(2\pi)^3}\int\frac{d\omega}{2\pi}\{M_q^{pl}[1-G_+(q)]\}^2D^{pl}(\mathbf{q},\omega)G(\mathbf{k}+\mathbf{q},k_0+\omega)\,, \tag{A3}$$

and Eq. (78) for $E_c^{pa}(k)$ is equivalent to

$$\Sigma_c^{pa}(\mathbf{k},k_0)=i\Omega\sum_\nu\int\frac{d^3q}{(2\pi)^3}\int\frac{d\omega}{2\pi}[M_q^{pa}G_-(q)]^2D_\nu^{pa}(\mathbf{q},\omega)G(\mathbf{k}+\mathbf{q},k_0+\omega)\,. \tag{A4}$$

Both of these expressions may be represented by the diagram shown in Fig. 7.

By defining the dynamical dielectric function (which we derive below),

$$\epsilon(\mathbf{q},\omega)=1+\frac{\omega_p^2}{[(\omega_q^{pl})^2-\omega_p^2]-\omega^2}\,, \tag{A5}$$

and using Eq. (15), we may rewrite Eq. (A3) as

$$\Sigma_c^{pl}(\mathbf{k},k_0)=i\int\frac{d^3q}{(2\pi)^3}\int\frac{d\omega}{2\pi}v(q)\left[\frac{1}{\epsilon(\mathbf{q},\omega)}-1\right][1-G_+(q)]^2G(\mathbf{k}+\mathbf{q},k_0+\omega)\,. \tag{A6}$$

This expression is an improved version, i.e., it includes the vertex correction $[1-G_+(q)]^2$, of the formula obtained by Quinn and Ferrell[29] for the density-induced correlation energy. Accordingly, as long as Eq. (A5) is deemed appropriate, the plasmon-pole term has the same structure as the "ordinary" method for calculating density-induced correlation effects. The vertex correction (included in our work) is quite important quantitatively.

The dynamical dielectric function $\epsilon(\mathbf{q},\omega)$, given by Eq. (A5), can be derived from the plasmon-pole model. Consider the effective dynamical interaction between two test charges imbedded in an electron liquid. By definition, the interaction should be

$$V_{tt}(\mathbf{q},\omega)\equiv\frac{V(q)}{\epsilon(\mathbf{q},\omega)} . \tag{A7}$$

On the other hand, in the plasmon-pole language the interaction is

$$V_{tt}(\mathbf{q},\omega)=V(q)+\frac{2\Omega\hbar_q^{\rm pl}(M_q^{\rm pl})^2}{(\hbar\omega)^2-(\hbar\omega_q^{\rm pl})^2} . \tag{A8}$$

The first term is the bare Coulomb interaction; the second term comes from virtual emission and absorption of plasmons by the two test charges. Equation (A5) is obtained by equating the right-hand sides of Eqs. (A7) and (A8), and using Eq. (15).

The dynamical dielectric function of the plasmon model is related to the static dielectric function $\epsilon(\mathbf{q},0)$ through Eq. (13). For example, for $q=0$,

$$\epsilon(0,\omega)=1-\frac{\omega_p^2}{\omega^2} ,$$

the exact Drude response of a classical Coulomb plasma. For $q\neq 0$, Eq. (A5) is also a good approximation at high frequencies.[30]

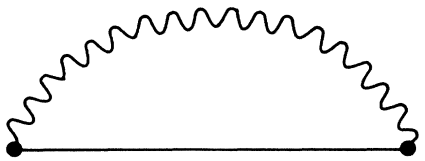

FIG. 7. Self-energy diagram corresponding to virtual emission and reabsorption of a plasmon (or paramagnon) by an electron. The two dots represent the electron-plasmon coupling $M_q^{\rm pl}[1-G_+(q)]$ or the electron-paramagnon coupling $M_q^{\rm pa}G_-(q)$.

In a similar way the dynamical spin susceptibility may be derived from the paramagnon-pole terms:

$$\chi(\mathbf{q},\omega)/\mu_B^2=-\frac{2\hbar\omega_q^{\rm pa}[M_q^{\rm pa}/V(q)]^2}{(\hbar\omega)^2-(\hbar\omega_q^{\rm pa})^2} . \tag{A9}$$

Equation (A4) can then be rewritten as

$$\Sigma_c^{\rm pa}(\mathbf{k},k_0)=-3i\int\frac{d^3q}{(2\pi)^3}\int\frac{d\omega}{2\pi}[G_-(q)V(q)]^2G(\mathbf{k}+\mathbf{q},k_0+\omega)\chi(\mathbf{q},\omega)/\mu_B^2 . \tag{A10}$$

If we replace $G_-(q)V(q)$ by a constant I, Eq. (A10) becomes the expression used by Doniach and Engelsberg[31] to calculate the paramagnon-induced self-energy in palladium. The factor 3 reflects the three components of the vector paramagnon, a multiplicity first emphasized by Penn.[32]

We have shown[10] that $G_-(q)V(q)$ is the irreducible interaction in the spin-antisymmetric channel, and is the cause of all the spin-induced correlation effects. Although effects of spin fluctuations were intensively studied in nearly ferromagnetic metals twenty years ago, they have been neglected in paramagnetic metals. The present paper has shown their importance in explaining the conduction-electron spectrum of simple metals.

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