Spin Susceptibility of an Interacting Electron Gas

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A simple calculation of the wave-vector- and frequency-dependent paramagnetic spin susceptibility of an interacting electron gas is presented. The equation of motion of the double-time Green's function is solved using a moment-conserving decoupling approximation. For the short-range interaction, our expression for the dynamic spin susceptibility reduces to a previous result of Wolff. In the static and long-wavelength limit, our result for the Stoner-enhanced spin susceptibility coincides with that obtained from consideration of the ground-state energy in the Hartree-Fock approximation.

I. INTRODUCTION

The free-electron model has proved very useful to understand, at least qualitatively, a number of important physical properties of simple metals. In this model the ion cores provide a uniform neutralizing background of positive charge and the conduction electrons are treated as a degenerate Fermi gas. The spin magnetism of the conduction electrons in simple metals can be correctly estimated from Pauli's formula. However, it is known for quite some time that one of the important manifestations of Coulomb interactions between the electrons is to enhance the spin susceptibility over Pauli's value.[1-4] In recent years, there has been renewed interest[3-6] to study the effect of electron-electron interaction on the properties of electron gas in metals. It is felt that a quantitative explanation of the Stoner-enhanced spin susceptibility of simple metals such as sodium, where the effect of periodic potential is known to be negligible, would provide a direct test of the theories of electron correlations at metallic densities.

Recently, Toigo and Woodruff[6] have developed a theory of dielectric response function of an interacting electron gas by solving the equation of motion for the Green's function of electron-density operators. These authors have used a moment-conserving decoupling approximation, suggested by Tahir-Kheli and Jarret.[7] The theory of Toigo and Woodruff[6] has given very good result for the dielectric function in the long-wavelength limit. It was, therefore, thought that it would be worthwhile to examine the spin susceptibility of an interacting electron gas in the same approximation.

In this paper we present a simple calculation of the wave-vector- and frequency-dependent paramagnetic spin susceptibility of an interacting electron gas. The equation of motion of the double-time Green's function is solved using a moment-conserving decoupling approximation. For the short-range interaction, our expression for the dynamic spin susceptibility reduces to a previous result of Wolff.[1] In the static and long-wavelength limit, our result for the Stoner-enhanced spin susceptibility coincides with that obtained from the consideration of the ground-state energy in the Hartree-Fock approximation.

II. GENERAL THEORY

The system of degenerate liquid of electrons, immersed in a uniform neutralizing background of positive charge is described by the Hamiltonian

$$H = H_0 + H_1 = \sum_{\vec{k},\sigma} \omega_{\vec{k}}\, a^{\dagger}_{\vec{k},\sigma}\, a_{\vec{k},\sigma} + \tfrac{1}{2} \sum_{\vec{k},\vec{k}\neq 0} \phi(\vec{k})\,(\rho_{\vec{k}}\rho^{\dagger}_{\vec{k}} - n)\,, \tag{1}$$

where $a^{\dagger}_{\vec{k},\sigma}$, $a_{\vec{k},\sigma}$ are the electron-creation and -annihilation operators, respectively, and $\omega_{\vec{k}} = k^2/2m$, $\phi(\vec{k}) = 4\pi e^2/k^2$. We use $\hbar = 1$ throughout. The Fourier transform of the electron-density-fluctuation operator is given by

$$\rho_{\vec{k}} = \sum_{\vec{q},\sigma} a^{\dagger}_{\vec{q},\sigma} a_{\vec{q}+\vec{k},\sigma} = \sum_{\vec{q},\sigma} \rho_{\vec{q},\sigma}(\vec{k})\,. \tag{2}$$

The Fourier transform of the z component of the spin-density-fluctuation operator is defined as

$$S_z(\vec{q}) = \tfrac{1}{2} \sum_{\vec{k},\sigma} \eta_\sigma\, \rho_{\vec{k},\sigma}(\vec{q}), \quad \eta_\sigma = \begin{cases} +1 & \text{for } \sigma = \uparrow \\ -1 & \text{for } \sigma = \downarrow \end{cases}\,. \tag{3}$$

The frequency- and wave-vector-dependent spin susceptibility is obtained as a linear response of an electron system to a magnetic disturbance. It may be expressed in terms of retarded Green's function as[8]

$$\begin{aligned} \chi(\vec{q},t) &= \langle\langle S_z(\vec{q},t);\, S^{\dagger}_z(\vec{q},0)\rangle\rangle \\ &= i\Theta(t)\langle \sum_{\vec{k},\sigma} \tfrac{1}{2}\eta_\sigma [\,\rho_{\vec{k},\sigma}(\vec{q},t),\, S^{\dagger}_z(\vec{q},0)]\rangle \\ &= \sum_{\vec{k},\sigma} \tfrac{1}{2}\eta_\sigma\, G_{\vec{k},\sigma}(\vec{q},t)\,, \end{aligned} \tag{4}$$

where the angular brackets denote the exact ground-state average, appropriate to the system Hamiltonian (1) and $\Theta(t)$ is the unit step function. We have defined the spin susceptibility in units of $g^2\mu_B^2$ where g is Lande's factor and μ_B is Bohr

magneton. It is possible now to derive the exact expressions for a few low-order frequency moments of the spin susceptibility function. To derive these moments we note that the imaginary part of this function is given by[9]

$$\chi''(\vec{q},t)=\tfrac{1}{2}\langle[S_z(\vec{q},t);S_z^\dagger(\vec{q},0)]\rangle \ . \tag{5}$$

We define the Fourier transform $\chi''(\vec{q},\omega)$ of the imaginary part of the spin susceptibility as

$$\chi''(\vec{q},t)=\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\,e^{-i\omega t}\,\chi''(\vec{q},\omega) \ . \tag{6}$$

The various odd frequency moments of $\chi''(\vec{q},\omega)$ can be obtained from Eq. (5), by differentiating it with respect to time and then taking the limit $t\to 0$. The resulting commutators can be exactly evaluated for the first few low-order moments. The first frequency moment is given by

$$\begin{aligned}\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\ \omega\chi''(\vec{q},\omega)&=\langle[[S_z(\vec{q},t),H],S_z^\dagger(\vec{q},0)]\rangle\\&=\frac{1}{4}\sum_{\vec{k},\sigma}(\omega_{\vec{k}+\vec{q}}-\omega_{\vec{k}})(n_{\vec{k},\sigma}-n_{\vec{k}+\vec{q},\sigma})\\&=\frac{nq^2}{4m} \ ,\end{aligned} \tag{7}$$

which is independent of particle interaction. However, in the third frequency moment, the Coulomb potential explicitly enters along with two-particle static correlation functions. The result for this moment shall not be given here. We shall make use of the first frequency moment to calculate the spin susceptibility of an interacting electron gas.

We derive an expression for the frequency- and wave-vector-dependent spin susceptibility by solving the equation of motion of Green's function occurring in Eq. (4). The equation of motion for the said Green's function is[8]

$$\begin{aligned}i\frac{d}{dt}\,G_{\vec{k},\sigma}(\vec{q},t)&=\delta(t)\langle[S_z(\vec{q}),\rho_{\vec{k},\sigma}(\vec{q})]\rangle\\&\quad+\langle\langle[\rho_{\vec{k},\sigma}(\vec{q}),H];S_z^\dagger(\vec{q})\rangle\rangle \ .\end{aligned} \tag{8}$$

Its Fourier transform is given by

$$\begin{aligned}G_{\vec{k},\sigma}(\vec{q},\omega)&=\frac{\eta_\sigma}{2}\,\frac{n_{\vec{k}+\vec{q},\sigma}-n_{\vec{k},\sigma}}{\omega-(\omega_{\vec{k}+\vec{q}}-\omega_{\vec{k}})}\\&\quad+\frac{\langle\langle[\rho_{\vec{k},\sigma}(\vec{q}),H_1];S_z^\dagger(\vec{q})\rangle\rangle_\omega}{\omega-(\omega_{\vec{k}+\vec{q}}-\omega_{\vec{k}})} \ .\end{aligned} \tag{9}$$

This is an exact equation and cannot be solved without making some approximation to linearize it. The commutator occurring in the last term of the above equation is found to be

$$\begin{aligned}&[\rho_{\vec{k},\sigma}(\vec{q}),H_1]\\&=\sum_{\vec{q}'}\phi(\vec{q}')\,(a_{\vec{k},\sigma}\rho_{\vec{q}'}a_{\vec{k}+\vec{q}-\vec{q}',\sigma}-a_{\vec{k}+\vec{q}',\sigma}\rho_{\vec{q}'}a_{\vec{k}+\vec{q},\sigma}) \ .\end{aligned} \tag{10}$$

Now if we make the usual Hartree–Fock-type decoupling approximation in Eq. (9), we obtain an integral equation

$$\begin{aligned}G_{\vec{k},\sigma}(\vec{q},\omega)&=\tfrac{1}{2}\eta_\sigma\,G^0_{\vec{k},\sigma}(\vec{q},\omega)+G^0_{\vec{k},\sigma}(\vec{q},\omega)\\&\quad\times\sum_{\vec{q}'}\phi(\vec{k}-\vec{q}')\,G_{\vec{q}',\sigma}(\vec{q},\omega) \ ,\end{aligned} \tag{11}$$

where

$$G^0_{\vec{k},\sigma}(\vec{q},\omega)=(n_{\vec{k}+\vec{q},\sigma}-n_{\vec{k},\sigma})/[\omega-(\omega_{k+q}-\omega_{\vec{k}})]$$

is the free-electron Green's function. Equation (11) is the same as obtained by Wolff.[1] The solutions of the above equation has been discussed by Wolff.[1]

However, here we make the following decoupling approximation:

$$\langle\langle[\rho_{\vec{k},\sigma}(\vec{q}),H_1];S_z^\dagger(\vec{q})\rangle\rangle_\omega=2A_{\vec{k},\sigma}(\vec{q})\,\langle\langle S_z(\vec{q});S_z^\dagger(\vec{q})\rangle\rangle_\omega \ . \tag{12}$$

Making use of Eqs. (12) and (9) in Eq. (4) we obtain

$$\chi(\vec{q},\omega)=\tfrac{1}{2}\,\chi_0(\vec{q},\omega)\Big/\left(1-\sum_{\vec{k},\sigma}\eta_\sigma\,\frac{A_{\vec{k},\sigma}(\vec{q})}{\omega-(\omega_{\vec{k}+\vec{q}}-\omega_{\vec{k}})}\right) \ , \tag{13}$$

where

$$\chi_0(\vec{q},\omega)=\frac{1}{2}\sum_{\vec{k},\sigma}\frac{n_{\vec{k}+\vec{q},\sigma}-n_{\vec{k},\sigma}}{\omega-(\omega_{\vec{k}+\vec{q}}-\omega_{\vec{k}})} \ . \tag{14}$$

The coefficient $A_{\vec{k},\sigma}(\vec{q})$ is determined by using the condition that the first frequency moments of both sides of Eq. (12) must be equal. This gives

$$A_{\vec{k},\sigma}(\vec{q})=\frac{1}{2}\,\frac{\langle[[[\rho_{\vec{k},\sigma}(\vec{q}),H_1],H],S_z^\dagger(\vec{q})]\rangle}{\langle[[S_z(\vec{q}),H],S_z^\dagger(\vec{q})]\rangle} \ . \tag{15}$$

The denominator here is obviously the exact first-frequency moment of the spin-susceptibility function, which we have already calculated [Eq. (7)]. For the evaluation of the numerator, we have made the usual Hartree-Fock decoupling approximation to calculate the averages. The contributions which are quadratic in interaction have been ignored here for simplicity. We hope to investigate the effects of these terms later. In the approximation described above, the numerator is given by

$$\begin{aligned}\langle[[[\rho_{\vec{k},\sigma}(\vec{q}),H_1],H],S_z^\dagger(\vec{q})]\rangle&=\tfrac{1}{2}\phi(\vec{q})(n_{\vec{k},\sigma}-n_{\vec{k}+\vec{q},\sigma})\\&\quad\times\sum_{\vec{q}_1,\sigma_1}\eta_{\sigma_1}(\omega_{\vec{q}_1+\vec{q}}-\omega_{\vec{q}_1})(n_{\vec{q}_1,\sigma_1}-n_{\vec{q}_1+\vec{q},\sigma_1})\\&\quad+\tfrac{1}{2}\eta_\sigma(n_{\vec{k},\sigma}-n_{\vec{k}+\vec{q},\sigma})\sum_{\vec{q}'}\phi(\vec{k}-\vec{q}')[(\omega_{\vec{k}+\vec{q}}-\omega_{\vec{k}})\\&\quad-(\omega_{\vec{q}'+\vec{q}}-\omega_{\vec{q}'})](n_{\vec{q}',\sigma}-n_{\vec{q}'+\vec{q},\sigma}) \ .\end{aligned} \tag{16}$$

On simplification it can be easily seen that the first term on right-hand side of above equation becomes

$$\tfrac{1}{2}\phi(\vec{q})(n_{\vec{k},\sigma}-n_{\vec{k}+\vec{q},\sigma})\,(q^2/m)(n\uparrow-n\downarrow) \ .$$

Now for the paramagnetic case $n\uparrow = n\downarrow = \frac{1}{2}n$ so that this term becomes zero. $A_{\vec{k},\sigma}(\vec{q})$ thus, can be evaluated and we obtain, for the paramagnetic spin susceptibility,

$$\chi(\vec{q},\omega) = \frac{1}{2}\,\frac{\chi_0(\vec{q},\omega)}{1 - I(\vec{q},\omega)\,\chi_0(\vec{q},\omega)}\ , \tag{17}$$

where

$$I(\vec{q},\omega) = \frac{1}{\chi_0(\vec{q},\omega)} \sum_{\vec{k},\sigma} P_{\vec{k},\sigma}(\vec{q})\,\frac{n_{\vec{k},\sigma} - n_{\vec{k}+\vec{q},\sigma}}{\omega - (\omega_{\vec{k}+\vec{q}} - \omega_{\vec{k}})} \tag{18}$$

and

$$P_{\vec{k},\sigma}(\vec{q}) = \frac{m}{nq^2} \sum_{\vec{q}'} \phi(\vec{k} - \vec{q}')[(\omega_{\vec{k}+\vec{q}} - \omega_{\vec{k}}) - (\omega_{\vec{q}'+\vec{q}} - \omega_{\vec{q}'})] \times (n_{\vec{q}',\sigma} - n_{\vec{q}'+\vec{q},\sigma})\ . \tag{19}$$

III. RESULTS

We shall now examine our expression for the frequency- and wave-vector-dependent spin susceptibility in the following important cases.

(*i*) *Wolff's case.* When the electron interaction is short ranged, i.e., $\phi(\vec{k} - \vec{q}') = v$ (a constant). In this case it can be easily seen that $P_{\vec{k},\sigma}(\vec{q})$ simplifies to $-\frac{1}{2}v$ and we get, from Eqs. (17) and (18),

$$\chi(\vec{q},\omega) = \frac{1}{2}\,\frac{\chi_0(\vec{q},\omega)}{1 - v\chi_0(\vec{q},\omega)}\ . \tag{20}$$

It is very interesting to note that this expression for spin susceptibility is exactly the same as obtained by Wolff[1] for the short-range interaction from Eq. (11).

(*ii*) *Static limit.* The second important case is to consider the expression (17) in the static limit (i.e., when $\omega \to 0$). In the static limit it can be seen that expression (17) reduces to

$$\chi(q,0) = \frac{1}{2}\,\frac{D(\epsilon_F)\,U(q,0)}{1 - I(q,0)\,D(\epsilon_F)\,U(q,0)}\ , \tag{21}$$

where $2D(\epsilon_F)$ is the density of states at the Fermi surface and

$$U(q,0) = \frac{1}{2} + \frac{1}{2q}\left(1 - \frac{q^2}{4}\right)\ln\left|\frac{q+2}{q-2}\right|\ . \tag{22}$$

In Eq. (21) and what follows q is expressed in units of q_F. $I(q,0)$ is the static limit of $I(q,\omega)$ and can be written in the form

$$I(q,0) = (8\pi e^2/q_F^2)\,G(q,0)/q^2\ , \tag{23}$$

where

$$G(q,0) = \frac{1}{2\phi(\vec{q})\,\chi_0(q,0)} \sum_{\vec{k},\sigma} P_{\vec{k},\sigma}(\vec{q})\,\frac{n_{\vec{k},\sigma} - n_{\vec{k}+\vec{q},\sigma}}{\omega_{\vec{k}} - \omega_{\vec{k}+\vec{q}}}\ , \tag{24}$$

which can be simplified to give

$$G(q,0) = -\frac{1}{2\phi(\vec{q})\,D(\epsilon_F)\,U(q,0)}\,\frac{2m(3\pi^2)}{q^2 q_F^3} \sum_{\vec{k},\vec{q}'} \phi(\vec{k} - \vec{q}') \times \left(1 - \frac{\omega_{\vec{q}'+\vec{q}} - \omega_{\vec{q}'}}{\omega_{\vec{k}+\vec{q}} - \omega_{\vec{k}}}\right)(n_{\vec{k}+\vec{q}} - n_{\vec{k}})(n_{\vec{q}'+\vec{q}} - n_{\vec{q}'})\ . \tag{25}$$

The integrals occurring in Eq. (23) are exactly the same as involved in the work of Toigo and Woodruff[6] and can be solved numerically by making certain transformations.[10]

(*iii*) *Stoner enhancement (long-wavelength limit).* It can be seen that in the long-wavelength limit (i.e., $q \to 0$) integrals occurring in Eq. (23) can be directly evaluated and one gets

$$\lim_{q\to 0}\,[G(q,0)/q^2] = \tfrac{1}{4}\ . \tag{26}$$

Also in the long-wavelength limit, $U(q,0)$ approaches unity. Thus, in the static and long-wavelength limit our expression for the paramagnetic spin susceptibility reduces to

$$\chi = \chi_0/(1 - \alpha)\ , \tag{27}$$

where χ_0 is the Pauli's paramagnetic spin susceptibility and

$$\alpha = (2\pi e^2/q_F^2)\,D(\epsilon_F) = 0.166\,r_s\ , \tag{28}$$

where r_s is the electron density parameter. The $(1 - \alpha)^{-1}$ is the factor by which the spin susceptibility is enhanced due to electron-electron interaction. It is very interesting to note that our result for Stoner-enhanced spin susceptibility coincides[11] with that obtained from consideration of the ground-state energy in the Hartree–Fock approximation.

The agreement of the enhanced paramagnetic susceptibility with experimental results on simple metals is not good. It is obvious from Eq. (28) which gives $\alpha = 0.66$ for $r_s = 4$. This value of r_s corresponds to metallic sodium. The experimental value[12] of α for sodium is 0.42. It is also known from the theory of Singwi *et al.*[4] that α does not depend linearly on r_s. It is more or less constant for entire metallic density range. The wave-vector dependence of the exchange-enhanced susceptibility is governed by the function $I(q)$. The importance of this function has been discussed in detail by Lowde and Windsor[13] and others.[14] We have plotted this function in Fig. 1. The q dependence of this function is the same as obtained by Toigo and Woodruff[6] in the case of dielectric function of an interacting electron gas. It is different from the q dependence obtained by Singwi *et al.*[4] These authors find that $I(q)$ has a gentle dependence on q, a result consistent with the experimental observations of Lowde and Windsor.[13]

IV. CONCLUDING REMARKS

The enhancement of paramagnetic susceptibility as predicted by Eqs. (27) and (28) is not in good agreement with experimental results. This may be due to following reasons. First, in the evaluation of the coefficient $A_{\vec{k},\sigma}(\vec{q})$ from Eq. (15) we have

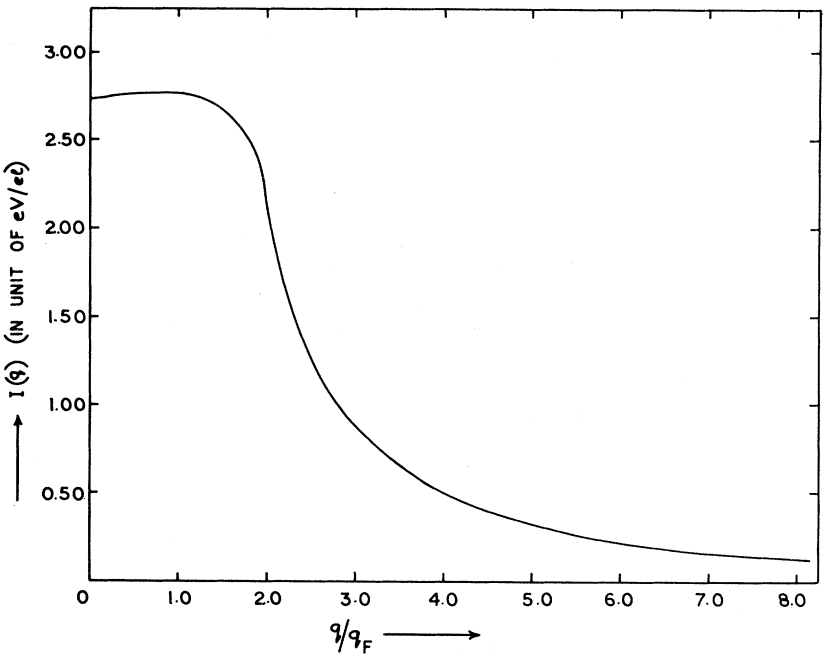

FIG. 1. Enhancement function $I(q)$ vs q for $r_s=4$.

ignored for simplicity the contributions which are quadratic in the interaction. It has been clearly demonstrated in this paper that the result then obtained in the static and long-wavelength limit coincides[11] exactly with the result obtained from consideration of the ground-state energy in Hartree–Fock approximation. This is one of the important conclusions of the present paper. The terms which are omitted in Eq. (15) will, therefore, give the explicit Coulomb correlation contributions. This will also modify the q dependence of $I(q)$ obtained here. Secondly, we have made use of simple Hartree–Fock decoupling approximation in calculating the averages involved in Eq. (15). Lastly, although the moment-conserving decoupling scheme of Toigo and Woodruff[6] has given reasonable result for the compressibility of an electron gas, this may not be a good approximation for the problem of spin susceptibility of an interacting electron gas. It is hoped that efforts will be made to clarify some of the points mentioned above.

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