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Self-Consistent Approximations for Itinerant Ferromagnetism Below the Phase-Transition Point

U. Brandt, H. Lustfeld, W. Pesch, and L. Tewordt

Abteilung für Theoretische Festkörperphysik
am Institut für Angewandte Physik der Universität Hamburg, Germany

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The self-consistent and "conserving" (in particular the total spin is conserved) approximation scheme, developed in a previous paper for itinerant ferromagnetism, is extended to the region below the phase-transition point. The former general condition for the transformation properties of any approximate self-energy part with regard to infinitesimal transformations in spin space is applied to the case where the transformation is a finite rotation in spin space; these rotations correspond to rotations of the direction of the spontaneous magnetization which is fixed here by an infinitesimal auxiliary field **H**. *This transformation property of the self-energy part ensures that the equations determining the corresponding Green's and correlation functions are covariant in form with respect to rotations of* **H**. *Two examples are considered: the "Hartree–Fock" and the "particle–hole* T*-matrix" approximations for the contact interaction or Hubbard model. In the first example the resulting susceptibilities are shown to be causal response functions, provided the Stoner equation is fulfilled. In the second example the self-energy part and the* T *matrix are discussed for the two cases where* **H** *is parallel and perpendicular to the axis of spin quantization. In fact, these expressions can be transformed into each other by means of the corresponding rotation matrix in spin space.*

1. INTRODUCTION

In a previous paper[1] a "self-consistent and conserving" approximation scheme for itinerant ferromagnetism was developed in analogy to the procedure of Baym and Kadanoff.[2] The main difference with regard to the latter work was the inclusion of an additional conservation law—the conservation law of the total spin of the many-particle system—into the approximation scheme. It turned out that this cannot simply be achieved by generalizing the theory of Ref. 2 because the spin variables have to be treated differently from the space–time variables. The fulfillment of the conservation law of the total spin of an itinerant ferromagnet led to severe restrictions for the possible approximations of the self-energy of the quasiparticles, and in consequence to severe restrictions for the possible approximations of the magnetic susceptibility.

In analogy to the work of Baym and Kadanoff[2] the method of Ref. 1 was based upon the equation of motion for the one-particle Green's function and

functional derivatives with respect to an external auxiliary potential (called U) yielding the appropriate correlation functions. The spin conservation law gave rise to a condition [Eq. (8) in Ref. 1] for the transformation properties of any approximate expression of the self-energy part with regard to infinitesimal transformations in spin space. It was shown that any approximate expression of the self-energy part given in terms of diagrams of the symmetrized technique of Abrikosov *et al.*[3] (where the interactions occur via four-point vertices) leads automatically to self-consistent and conserving approximations. This in general is not the case for approximate expressions given by diagrams of the usual kind where the two-body interactions are described by interaction lines.

In the first part of this paper the general theory of Ref. 1 is extended to the region below the phase-transition point where a spontaneous magnetization occurs. The general considerations and equations of Ref. 1, in particular those regarding the consequences of the conservation law of the total spin, remain valid. However, there exists an important difference between the solutions of the general equations for the paramagnetic and ferromagnetic regions: in contrast to the solution for the paramagnetic region the solution for the ferromagnetic region depends on the way $\lim U \to 0$ is carried out. In the latter case the auxiliary potential U is first taken to be the one describing the energy of the magnetic moments of the electrons in the presence of a constant magnetic field having the required direction of the spontaneous magnetization, and then the amplitude of this field is considered to tend to zero. This type of limiting procedure is discussed extensively by Mattuck.[4]

The physical meaning of the solution, for instance, of the self-energy part or the magnetic susceptibility must not depend on the direction of the spontaneous magnetization (given by the direction of the auxiliary infinitesimal field $\mathbf{H}$) with respect to the axis of the quantization of the spins of the electrons (the latter axis is taken here to be always the z axis). It is just the aforementioned condition for the transformation properties of the self-energy part [Eq. (8) of Ref. 1] which guarantees that these physical requirements are also satisfied in approximate calculations. To fulfill these physical requirements we shall construct in this paper the approximate self-energy parts by means of the symmetrized diagram technique of Abrikosov *et al.*[3]

As an example of a self-consistent and conserving approximation scheme the Hartree–Fock approximation for the contact interaction and the Hubbard model was discussed in Ref. 1. In the second part of this paper the corresponding equations, given in Ref. 1 are solved for the ferromagnetic region. The resulting expressions for the transverse and longitudinal susceptibilities, $\chi(q, \omega)$, agree with those which have been derived formerly by Kubo *et al.*[5] It is shown that at least at zero temperature these expressions of $\chi(q, \omega)$ have the correct analytic properties in the complex ω plane which must hold for any causal response function. This is true if the magnetization M and the coupling constant V are related by the Stoner equation which is just the self-consistency condition of the Hartree–Fock approximation. For values of the coupling constant V exceeding a certain critical value at a given magnetization $V_{cr}(M)$ [where $V_{cr}(M) \geq V_{\text{Stoner}}(M)$ always], the Hartree–Fock expressions of the susceptibilities have a singularity in the upper half of

the complex ω plane. Further, the dispersion laws of the two collective modes obtained from the transverse and longitudinal susceptibilities are discussed.

The equations determining the Green's function and susceptibility of the ferromagnetic state in the Hartree–Fock approximation can easily be generalized to the corresponding ones determining these quantities for the state of a spiral spin density wave of wave number, say, Q. In the limit $Q \to 0$ the Green's function tends to that of the ferromagnetic state having its magnetization directed along the x axis; this Green's function has also off-diagonal components with respect to the spin indices. The components of the Fourier transform of the correlation function have to be determined from a system of 16 linear algebraic equations which can be reduced and solved easily only in the limit $Q \to 0$. Our approximate calculation of the correlation function is a generalization of that given by Fedders and Martin[6] ensuring the covariance of the equations with respect to rotations of $\mathbf{Q}$.

In the third part of this paper the equations of Ref. 1 determining the self-energy part for the contact interaction and Hubbard model in the so-called "particle–hole T-matrix approximation" are discussed for the ferromagnetic region. To give an example of the covariance of this approximation scheme the expressions of the T matrix and self-energy part are determined for the two cases where the infinitesimal auxiliary field $\mathbf{H}$ is directed along the z and x axes. It turns out that, in fact, these quantities can be transformed into each other by means of the corresponding rotation in spin space. Brinkman and Engelsberg[7] have previously derived these expressions of the self-energy part and T matrix in the case where the magnetization is parallel to the z axis; then the evaluation of the equations determining the T matrix becomes most simple. Johansson[8] has looked for the poles of the T matrix in the case where the magnetization is parallel to the x axis. From our transformation relation it can be seen immediately that the poles coincide in both cases; it follows also that the expressions of the "exchange splitting energy" are identical.

So far the equations determining the correlation function, and thus the susceptibility, in the particle–hole T-matrix approximation have not been solved for the paramagnetic region, not to speak of the ferromagnetic region. It is desirable to persue this problem further because recently there have been extensive neutron-scattering experiments on Fe and Ni,[9] in particular in the phase-transition region, showing some yet unexplained features.

2. EXTENSION OF THE APPROXIMATION SCHEME TO $T < T_c$

The itinerant ferromagnetism is described in second quantization by the following Hamiltonian:

$$\begin{aligned}\mathscr{H} = &\int \psi_\alpha^+(r) h_0(r) \psi_\alpha(r)\, d^3r \\ &+ \int \psi_\alpha^+(r_1)\psi_\beta^+(r_2) V(r_1, r_2)\psi_\beta(r_2)\psi_\alpha(r_1)\, d^3r_1\, d^3r_2 \\ &+ \int \psi_\alpha^+(r_1, \tau_1) U_{\alpha\beta}(r_1, \tau_1; r_2, \tau_2)\psi_\beta(r_2, \tau_2)\, d^3r_1\, d^3r_2\, d\tau_1\, d\tau_2\end{aligned} \tag{1}$$

where V is the two-body interaction potential and U is an external auxiliary potential. It is always summed over repeated spin variables α, β, etc.; $\alpha = +(\uparrow)$ and $-(\downarrow)$, and the integrations over the time variables τ_1, τ_2, etc., are always taken from zero to T^{-1} (T is the temperature). The one-particle Green's function G satisfies, then, the following equation of motion:

$$\int [(G^0_{\alpha\gamma}(1, 2))^{-1} - U_{\alpha\gamma}(1, 2)]G_{\gamma\beta}(2, 1'; U)\, d2 = \delta(1 - 1')\delta_{\alpha\beta} + \int \Sigma_{\alpha\gamma}(1, 2)G_{\gamma\beta}(2, 1'; U)\, d2 \tag{2}$$

where Σ is the self-energy part. The arguments 1, 1', 2, etc., denote space and time variables. At the end of the calculation the Green's function, the self-energy part, and all the other quantities are taken for the limit $U \to 0$. Contrary to the solutions for the paramagnetic region the limits of these solutions for the ferromagnetic region are not unique. This is due to the fact that the direction of the spontaneous magnetization is arbitrary for this model of an itinerant ferromagnet. In order to obtain a spontaneous magnetization in a certain direction one carries out the limiting procedure $U \to 0$ in two steps. First, U is specialized to describe the interactions of the magnetic moments of the particles with a constant homogeneous magnetic field $\mathbf{H}$ having the required direction of the magnetization; then the third part of the Hamiltonian in Eq. (1) becomes equal to

$$\int \psi^+_\alpha(r)[-\tfrac{1}{2}g\mu_\beta \boldsymbol{\sigma}_{\alpha\beta} \cdot \mathbf{H}]\psi_\beta(r)\, d^3r \tag{3}$$

where the components σ^x, σ^y, σ^z of the vector $\boldsymbol{\sigma}$ are the Pauli spin matrices. In the second step of the limiting procedure the amplitude of $\mathbf{H}$ is let to go to zero. In this way one selects one of the infinite number of solutions, i.e., that giving rise to a spontaneous magnetization in the direction of $\mathbf{H}$. In all cases where the infinitesimal auxiliary field $\mathbf{H}$ is not parallel to the z axis the 2×2 matrices $G_{\alpha\beta}$ and $\Sigma_{\alpha\beta}$ have off-diagonal elements being different from zero.

The physical predictions obtained from the solution of the equation of motion for the Green's function, Eq. (2), must not depend on the direction of the auxiliary field $\mathbf{H}$. That means Eq. (2) has to be covariant in form with respect to a rotation of $\mathbf{H}$. Since, according to the form of $U_{\alpha\beta}$ [that is the term in square brackets in Eq. (3)], a rotation of $\mathbf{H}$ leads to an equivalent one in spin space one concludes that Eq. (2) has also to be covariant in form with respect to the latter rotation in spin space.

In order to fulfill these covariance requirements with respect to rotations of the auxiliary field $\mathbf{H}$ also in approximate calculations, one chooses an approximate expression for the self-energy part which satisfies the conditions 1, 2, and 3 stated in Ref. 1. The first condition says that $\Sigma_{\alpha\beta}$ has to be a functional of G and V only; the dependence on U arises only via G. The third condition is a condition for the transformation properties of the approximate self-energy part with respect

to infinitesimal transformations in spin space, i.e.,

$$\begin{aligned}\Sigma_{\alpha\beta}[1,1';(\delta_{\gamma\delta}-i\Lambda_{\gamma\delta}(2))G_{\delta\eta}(2,2')(\delta_{\eta\xi}+i\Lambda_{\eta\xi}(2'))]\\ =(\delta_{\alpha\delta}-i\Lambda_{\alpha\delta}(1))\Sigma_{\delta\eta}[1,1';G_{\gamma\xi}(2,2')](\delta_{\eta\beta}+i\Lambda_{\eta\beta}(1'))\end{aligned} \tag{4}$$

where $\Lambda_{\alpha\beta}(1)$ is an arbitrary infinitesimal tensor field. For the special case of an infinitesimal transformation corresponding to an infinitesimal rotation of **H** the components of the tensor field $\Lambda_{\alpha\beta}$ are infinitesimal constants. In that case Eq. (4) can be integrated to yield the transformation relation corresponding to a *finite* rotation of H. In shorthand notation this generalized relation reads as follows:

$$\Sigma(G_T)=\Sigma_T(G) \tag{5}$$

where the subscript T means "transformed quantity." Now one can show easily by means of the relation in Eq. (5) that indeed the equation of motion for the Green's function [Eq. (2)] is covariant in form with respect to a rotation of **H**. It should be stressed that according to our derivation this is true also for the equation of motion containing the approximate Green's function and self-energy part, provided the latter satisfies the condition (4).

The so-called two-particle correlation function L is defined by

$$L_{\alpha\beta\gamma\delta}(1,2,1',2')=-\frac{\delta G_{\alpha\gamma}(1,1')}{\delta U_{\delta\beta}(2',2)}\bigg|_{U\to 0} \tag{6}$$

The limiting procedure $U\to 0$ in Eq. (6) has to be carried out in the same way as has been described above. The correlation function L can also be calculated from an integral equation, i.e.,

$$\begin{aligned}L_{\alpha\beta\gamma\delta}(1,2,1',2')=&-G_{\alpha\delta}(1,2')G_{\beta\gamma}(2,1')+\int G_{\alpha\zeta}(1,3)\\ &\times G_{\eta\gamma}(3',1')\Gamma^1_{\zeta\nu\eta\kappa}(3,4',3',4)L_{\kappa\beta\nu\delta}(4,2,4',2')\,d2\,d3'\,d4\,d4'\end{aligned} \tag{7}$$

where G is taken for the limit $U\to 0$ and the "irreducible-vertex part" Γ^1 is given by

$$\Gamma^1_{\alpha\beta\gamma\delta}(1,2,1',2')=\frac{\delta\Sigma_{\alpha\gamma}(1,1')}{\delta G_{\delta\beta}(2',2)}\bigg|_{U\to 0} \tag{8}$$

Again the limits $U\to 0$ in G of Eq. (7) and on the right-hand side of Eq. (8) have to be carried out in the way described above. The correct, and thus also the approximate, Γ^1 has to satisfy a certain symmetry relation with respect to its arguments [see Eq. (7) in Ref. 1]. According to Eq. (8) this leads to a further condition for the acceptable approximations of Σ. This condition is the aforementioned condition 2.

It can be shown that the Eq. (7) for the correlation function L is, like the equation of motion for G, covariant in form with respect to a rotation of the auxiliary field **H** which is, as was stated above, equivalent to a certain transformation in spin space. For the proof one needs a relation between the transformed

Γ^1 and the transformed right-hand side of Eq. (8) which reads as follows (subscript T means, again, "transformed quantity"):

$$\Gamma_T^1 = \left(\frac{\delta\Sigma(G)}{\delta G}\right)_T = \frac{\delta\Sigma(G_T)}{\delta G_T} \tag{9}$$

The relation (9) can be derived with the help of the condition in Eq. (5) for the transformation property of the approximate expression of the self-energy part.

In analogy to the procedure described in Ref. 1 a generalized differential conservation law can be derived which reads as follows:

$$\begin{aligned} i\frac{\partial}{\partial\tau_2}L_{\alpha\beta\gamma\delta}(1,2,1',2) + \nabla_2\left(\frac{\nabla_2 - \nabla_2'}{2im}\right)L_{\alpha\beta\gamma\delta}(1,2,1',2')|_{2'\to 2} \\ = -[\delta(2-1)\delta_{\alpha\delta}G_{\beta\gamma}(2,1') - \delta(1'-2)\delta_{\beta\gamma}G_{\alpha\delta}(1,2)] \end{aligned} \tag{10}$$

For the paramagnetic region Eq. (10) goes over into Eq. (10) in Ref. 1 because the Green's function then has only equal diagonal components.

From the correlation function the transverse and longitudinal susceptibilities of wave number q and imaginary frequency $i\nu_m = i2m\pi T$ (the m's are all integers) are obtained by means of the following equations:

$$\begin{aligned} \chi^{\pm}(q, i\nu_m) &= \mathrm{FT}\{L_{+--+}(1,1',1,1')\} \\ \chi^{\mp}(q, i\nu_m) &= \mathrm{FT}\{L_{-++-}(1,1',1,1')\} \\ \chi^{zz}(q, i\nu_m) &= \tfrac{1}{4}\mathrm{FT}\{L_{\alpha\beta\gamma\delta}(1,1',1,1')\sigma_{\alpha\gamma}^z\sigma_{\beta\delta}^z\} \end{aligned} \tag{11}$$

where the abbreviation FT means the Fourier transform with respect to space and time variables [compare Eqs. (13) and (14) in Ref. 1]. Notice that below T_c the transverse (superscripts $\pm$ and $\mp$) and longitudinal (superscripts zz) susceptibilities become different.

In analogy to Ref. 1 it can be shown with the help of Eq. (10) that also the approximate dynamical ($\omega > 0$) susceptibilities are in accordance with the general relation:

$$\omega\chi^{\alpha\beta}(q=0,\omega) = \int d^3r[S^{\alpha}(\mathbf{r},0), S^{\beta}(0,0)] \qquad \text{for } \alpha,\beta = +_1 - {}_1z \tag{12}$$

The conditions stated in Eq. (12) become all important in the vicinity of the phase-transition point because then $\chi(q,\omega)$ has a critical behavior for small arguments. The fulfillment of the conditions in Eq. (12) can be ensured, as follows from the foregoing discussion, by choosing at the start an approximate Σ in accordance with Eq. (4), and then calculating Γ^1 from this Σ with the help of Eq. (8), and finally solving Eq. (7), containing this approximate Γ^1, and inserting the resulting L into Eq. (11).

3. THE HARTREE–FOCK APPROXIMATION

In this and the following sections the two-body interaction potential V in the Hamiltonian Eq. (1) is specialized to a delta-function potential of strength V,

or to the potential of the Hubbard model describing narrow-band ferromagnetism. In the latter model only the interactions between electrons hopping into Wannier states at the same atom are taken into account. It was shown in Ref. 1 that the symmetrized diagram technique of Abrikosov *et al.*[3] leads automatically to self-consistent and conserving approximations. For the model of contact interactions this means the contribution of any self-energy diagram constructed from four-point vertices Γ^0, given by

$$\Gamma^0_{\alpha\beta\gamma\delta}(1, 2, 3, 4) = V(\delta_{\alpha\gamma}\delta_{\beta\delta} - \delta_{\alpha\delta}\delta_{\beta\gamma})\delta(1 - 2)\delta(3 - 1)\delta(2 - 4) \tag{13}$$

and dressed Green's functions G satisfies Eq. (4).

The most simple self-energy diagram containing only one vertex part Γ^0 (drawn as a square) yields a contribution

$$\Sigma^{\mathrm{HF}}_{\alpha\beta}(1, 1') = -\int \Gamma^0_{\alpha\mu\nu\beta}(1, 2, 3, 1')G^{\mathrm{HF}}_{\nu\mu}(3, 2)\, d3\, d2 \tag{14}$$

According to our approximation scheme described in Section 2 the corresponding correlation function L, and thus the susceptibility χ, is obtained by inserting Eq. (14) into Eq. (8) and using the resulting Γ^1 as the kernel in Eq. (7) for L. The whole approximation scheme is called the Hartree–Fock approximation.

The calculations become most easy if the direction of the auxiliary infinitesimal field **H** is chosen along the z direction. Then the Green's function, and accordingly the self-energy part, have no off-diagonal components. The Fourier transforms of the diagonal components of Σ become, according to Eq. (14) and the definition of the Green's function constants,

$$\Sigma^{\mathrm{HF}}_{++}(k, i\omega_n) = VN_-/\Omega \qquad \Sigma^{\mathrm{HF}}_{--}(k, i\omega_n) = VN_+/\Omega \tag{15}$$

where $\omega_n = (2n + 1)\pi T$, Ω is the volume of the crystal, and $N_\pm$ denote the total numbers of quasi particles having spin up or down, respectively. In the following calculations the crystal potential occurring in the one-body part h_0 of the Hamiltonian Eq. (1) is neglected. Then the energies of the quasiparticles of momentum k and spin up or down, which are given by the poles of the Fourier transforms of the Green's functions containing the self-energy parts in Eq. (15), become equal to

$$E^{\mathrm{HF}}_\pm(k) = \frac{k^2}{2m} + V\frac{N_\mp}{\Omega} - \mu \tag{16}$$

As usual these energies are measured relative to the chemical potential μ. The two Fermi spheres corresponding to the numbers $N_\pm$ of particles have radii equal to (at zero temperature)

$$k_\pm = (6\pi^2 N_\pm/\Omega)^{1/3} \tag{17}$$

The relative magnetization M can be expressed in terms of these radii by means of

$$M \equiv \frac{N_+ - N_-}{N_+ + N_-} = \frac{k_+^3 - k_-^3}{k_+^3 + k_-^3} \tag{18}$$

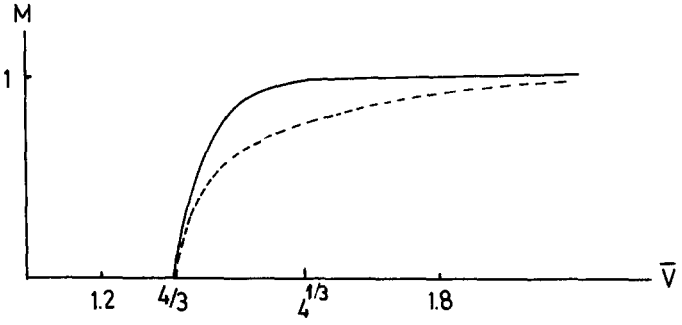


Fig. 1. Solid line: the relative magnetization M, calculated from the Hartree–Fock self-consistency condition Eq. (19) (Stoner equation), is plotted vs. the reduced coupling constant $\bar{V}$ [Eq. (20)]. The total ferromagnetic state, $M = 1$, is reached at $\bar{V} = 4^{1/3}$. Dashed line: maximum of the allowed values of the coupling constant, $\bar{V}_{cr}(M)$ [from Eq. (27)], for the longitudinal Hartree–Fock susceptibility [Eq. (23)]; for $\bar{V} \geq \bar{V}_{cr}$ at a given M this susceptibility becomes nonanalytic in the upper half of the complex frequency plane. The corresponding "critical curve" for the transverse susceptibility [Eq. (22)] is identical to the Stoner curve (solid line).

Since the quasi particle energies $E_{\pm}^{\mathrm{HF}}(k)$ are measured relative to μ their expressions, given in Eq. (16), have to vanish at $k = k_{\pm}$. Setting the resulting two conditions equal and expressing the quantities $k_{\pm}$ with the help of the relations (17) and (18) in terms of M one finds the well-known Stoner equation (valid at zero temperature)

$$\bar{V} = (M)^{-1}[(1 + M)^{2/3} - (1 - M)^{2/3}] \tag{19}$$

Here the dimensionless coupling constant $\bar{V}$ is defined by

$$\bar{V} = [2m/(3\pi^2)^{2/3}](N/\Omega)^{1/3} \tag{20}$$

where N is the total number of electrons. In Fig. 1 the relative magnetization M, calculated from the Stoner equation (19) in dependence of $\bar{V}$, is plotted vs. this dimensionless coupling constant $\bar{V}$.

Inserting now the Hartree–Fock self-energy part, given in Eq. (14), into the Eq. (8), one finds for the irreducible vertex part in this approximation

$$\Gamma^1_{\mathrm{HF}} = \Gamma^0 \tag{21}$$

Thus, the kernel Γ^1 occurring in the Eq. (7) for L has to be approximated by Γ^0. Then this equation can easily be solved by Fourier transformation. The corresponding susceptibilities are obtained with the help of Eq. (11), the results being equal to

$$\chi^{\pm}_{\mathrm{HF}}(q, iv_m) = \frac{\chi^0_{+-}}{1 - V\chi^0_{+-}} \tag{22}$$

$$\chi^{zz}_{\mathrm{HF}}(q, iv_m) = \frac{1}{4}\frac{\chi^0_{++} + \chi^0_{--} + 2V\chi^0_{++}\chi^0_{--}}{1 - V^2\chi^0_{++}\chi^0_{--}} \tag{23}$$

In the expressions of Eqs. (22) and (23) the following abbreviations have been used:

$$\chi^0_{\alpha\beta}(q, iv_m) = -T \sum_{i\omega_n} \int \frac{d^3k}{(2\pi)^3} G^{\mathrm{HF}}_{\alpha\alpha}(k + q, i\omega_n + iv_m) G^{\mathrm{HF}}_{\beta\beta}(k, i\omega_n) \tag{24}$$

The expression for $\chi^{\mp}_{\mathrm{HF}}$ is obtained from that in Eq. (22) by interchanging $+$ and $-$. The expressions of the susceptibilities given in the Eqs. (22)–(24) agree with those which have been derived previously by Kubo *et al.*[5] by means of the random-phase approximation in the equation of motion. Now it has been shown that the Kubo susceptibility is intimately connected to the Hartree–Fock approximation of the self-energy part, given in Eq. (14).

It is plausible to ask whether or not the self-consistent and conserving approximation scheme described in Section 2 leads automatically to an approximate expression of $\chi(q, \omega)$ being an analytic function of ω in the upper half of the complex ω plane, as it must be on general theoretical grounds for any causal response function. It will be shown in the following that this is indeed so in the Hartree–Fock approximation. However, we have not succeeded to give a general proof that our self-consistent and conserving approximation leads always to causal response functions. Since the functions $\chi^0_{\alpha\beta}(q, \omega)$ are analytic functions in the upper half of the complex ω plane one has to look for zeros of the denominators of the expressions in Eqs. (22) and (23). In the appendix it is shown by using an idea of Pines and Nozières[10] that the following inequalities ensure the analyticity of the Hartree–Fock susceptibilities (22) and (23):

$$1 - V\chi^0_{+-}(q, 0) \geq 0 \tag{25}$$

$$1 - V^2\chi^0_{++}(q, 0)\chi^0_{--}(q, 0) \geq 0 \tag{26}$$

It should be noted that these conditions are valid also for general noninteracting particle energies $\varepsilon(k)$ occurring instead of $k^2/2m$ in Eq. (16), and thus in Eqs. (22)–(24).

For a further examination of the analyticity conditions, stated in Eqs. (25) and (26), we specialize to the case of zero temperature and $\varepsilon(k) = k^2/2m$. Then it suffices to examine these inequalities for $q = 0$ because $\chi^0_{\alpha\beta}(q, 0)$ has a maximum at $q = 0$. It is clear that by increasing V the left-hand sides of Eqs. (25) and (26) eventually become zero. The corresponding "critical" values of $\overline{V}$ are denoted by $\overline{V}_{cr}$; they depend via $k_{\pm}$ on the magnetization M: $\overline{V}_{cr} = \overline{V}_{cr}(M)$. From Eq. (25) one finds that the critical curve for the transverse susceptibility is identical with the Stoner curve shown in Fig. 1, while Eq. (26) yields the relation for the longitudinal susceptibility:

$$\overline{V}_{cr} = \tfrac{4}{3}(1 - M^2)^{-1/6} \tag{27}$$

The resulting critical curve $M(V_{cr})$ is also shown in Fig. 1. Thus, one finds that for both susceptibilities the critical values of the coupling constant (larger values of $\overline{V}$ make these susceptibilities nonanalytic) satisfy at a given M the following inequality:

$$\overline{V}_{\mathrm{Stoner}}(M) \leq \overline{V}_{cr}(M) \tag{28}$$

Here $\bar{V}_{\text{Stoner}}$ means the value of the coupling constant calculated from the Stoner equation (19). Recall that the latter relation makes the Hartree–Fock approximation a self-consistent approximation. Thus, the inequality in Eq. (28) says that both susceptibilities, given in Eqs. (22) and (23), are causal response functions, provided that the Stoner equation is satisfied.

A pole of the susceptibility $\chi(q, \omega)$ on the real axis of the complex ω plane, denoted by $\omega_0(q)$, corresponds to a collective mode. The expression of the transverse susceptibility in Eq. (22) yields the spin wave having the dispersion law

$$\omega_0 = (2m)^{-1} F(M) q^2 \quad \text{for } q \ll k_+ \tag{29}$$

where the function $F(M)$ is monotonically increasing from zero to $\frac{1}{5}$ as M increases from 0 to 1 and has a vanishing slope at $M = 1$. The expression of the longitudinal susceptibility in Eq. (23) yields a collective mode of the zero-sound type; we find a dispersion law of the form (in the limit $M \to 1$ this mode vanishes in the continuum of the particle–hole excitations)

$$\omega_0 \simeq m^{-1} k_+ q \quad \text{for } q \ll k_+ \tag{30}$$

Now we turn to the Hartree–Fock approximation for the state of a spiral spin-density wave of wave number Q. The auxiliary field is assumed to rotate in the xy plane as z increases according to

$$H_x + iH_y = He^{iQz} \tag{31}$$

This auxiliary field produces a rotating magnetization of amplitude MN/Ω behaving in the same way as the auxiliary field in Eq. (31). The Hartree–Fock self-consistency condition of Σ is again given by Eq. (14). This equation, together with the equation of motion for G in Eq. (2), yields the following Fourier transforms of the components of G of wave number k and frequency $i\omega_n$:

$$G^{\text{HF}}_{\pm\pm}(k, i\omega_n; Q) = \frac{1}{2}(g_+ + g_-) \pm \frac{1}{4} \frac{[\varepsilon(k+Q) - \varepsilon(k)]}{A(k, Q)} (g_+ - g_-)$$

$$G^{\text{HF}}_{\pm\mp}(k, i\omega_n; Q) = \frac{1}{2}\left(\frac{VNM}{2\Omega}\right)(A(k, Q))^{-1}(g_+ - g_-) \tag{32}$$

Here we have used the abbreviations

$$g_\pm(k, i\omega_n; Q) = [i\omega_n - E^{\text{HF}}_\pm(k, Q)]^{-1} \tag{33}$$

where the quasiparticle energies are given by

$$E^{\text{HF}}_\pm(k, Q) = \tfrac{1}{2}[\varepsilon(k+Q) + \varepsilon(k)] \mp A(k, Q) - \mu \tag{34}$$

$$A(k, Q) = \left\{ \tfrac{1}{4}[\varepsilon(k+Q) - \varepsilon(k)]^2 + \left[\frac{VNM}{2\Omega}\right]^2 \right\}^{1/2} \tag{35}$$

For brevity we omit the generalized Stoner equation relating the amplitude MN/Ω of the spiral spin-density wave and the coupling constant V. It should be remarked that in the case where only one energy band is involved such a state can be stable only if $\varepsilon(k)$ is not of the parabolic form.

In the limit $Q \to 0$ the expressions of the Green's functions in Eq. (32) tend to those of the ferromagnetic state having a magnetization M directed along the x axis. The "exchange splitting of the bands," given by the difference $[E_+^{\mathrm{HF}}(k, 0) - E_-^{\mathrm{HF}}(k, 0)]$ of the expressions in Eq. (34), turns out to be equal to the one obtained from the quasiparticle energies in Eq. (16), valid when M is directed along the z axis; this must be so because the Hartree–Fock approximation is self-consistent in the sense of Section 2 and therefore covariant with respect to rotations of the magnetization **M**. In the limit $M \to 0$ the Eq. (32) yields $G_{++}^{\mathrm{HF}} \to G^0(k, i\omega_n)$, $G_{--}^{\mathrm{HF}} \to G^0(k + Q, i\omega_n)$, and the off-diagonal components tend to zero.

In the Hartree–Fock approximation for the spiral spin-density wave the kernel Γ^1 occurring in the integral equation (7) for the correlation function L has to be approximated by Γ^0. Fourier transformation of Eq. (7) leads to a system of linear algebraic equations for the 16 components $L_{\alpha\beta\gamma\delta}^{\mathrm{HF}}(q, iv_m; Q)$ of the correlation function, the coefficients being equal to

$$A_{\alpha\beta\gamma\delta}(q, iv_m; Q) = T \sum_{i\omega_n} \int \frac{d^3k}{(2\pi)^3} G_{\alpha\beta}^{\mathrm{HF}}(k + q, i\omega_n + iv_m; Q) G_{\gamma\delta}^{\mathrm{HF}}(k, i\omega_n; Q) \quad (36)$$

Equations (32)–(36) have been derived previously[11] for the model of an antiferromagnetic chain. In the three-dimensional case there are nine different types of coefficients A; therefore, it is not possible to transform the expressions for the solutions of the components of L, which are given by Kramer's rule in terms of the A's, into simple expressions as is the case in the limit $Q \to 0$.

The calculation of Fedders and Martin[6] for the two-band model of an itinerant antiferromagnet differs from the one given above essentially in that they have taken into account only that scattering channel of Γ^0 leading to the "ladder part" of L. Thus, their equation for L is not covariant with respect to rotations of **Q**. It is likely that the complete system of equations for the sixteen components of the Fourier transform of L will give rise to several collective modes, one being the spin wave with a soundlike dispersion law.[6]

4. PARTICLE-HOLE T-MATRIX APPROXIMATION

The sum of all the contributions of self-energy diagrams containing $1, 2, \ldots$ vertices Γ^0 in a chain yields the expression

$$\Sigma_{\alpha\beta}^T(1, 1') = -\int T_{\alpha\gamma\lambda\beta}(1, 2, 3, 1') G_{\lambda\gamma}^T(3, 2)\, d3\, d2 \quad (37)$$

where the T matrix has to be determined from the integral equation

$$T_{\alpha\beta\gamma\delta}(1, 2, 3, 4) = \Gamma_{\alpha\beta\gamma\delta}^0(1, 2, 3, 4) + \int \Gamma_{\alpha\mu\gamma\nu}^0(1, 2', 3, 4') \times G_{\nu\lambda}^T(4, 1') G_{\kappa\mu}^T(3, 2') T_{\lambda\beta\kappa\delta}(1', 2, 3', 4)\, d1'\, d2'\, d3'\, d4' \quad (38)$$

Now we specialize U again to describe the energy of the electrons in the presence

of an infinitesimal auxiliary field **H**. Then Eq. (38) for T is covariant in form with respect to a rotation of **H**, as can be shown in an analogous way as has been done for Eq. (7) determining L. The Fourier transformation of Eq. (37) yields

$$\Sigma^T_{\alpha\beta}(k, i\omega_n) = -T\sum_{i\zeta_n}\int \frac{d^3p}{(2\pi)^3} T_{\alpha\gamma\lambda\beta}(k - p, i\omega_n - i\zeta_n) G^T_{\lambda\gamma}(p, i\zeta_n) \tag{39}$$

First, **H** is chosen to be directed along the z axis. Then the matrix $G^T_{\alpha\beta}$ becomes diagonal; this is true for any approximate Green's function provided Eqs. (2) and (4) are satisfied. Equation (38) can be transformed by Fourier transformation into a system of linear algebraic equations for the components of T. Then the expressions of those components of T which are needed to calculate the self-energy part according to Eq. (39) turn out to be

$$\begin{aligned} T^z_{++++}(q, iv_m) &= -\frac{V^2\chi_{--}}{1 - V^2\chi_{++}\chi_{--}} \\ T^z_{+--+}(q, iv_m) &= -\frac{V}{1 - V\chi_{+-}} \end{aligned} \tag{40}$$

where the superscripts z mean that **H** is along the z axis and where the $\chi_{\alpha\beta}$ are equal to

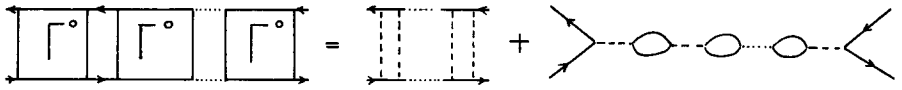
$$\chi_{\alpha\beta}(q, iv_m) = -T\sum_{i\omega_n}\int \frac{d^3k}{(2\pi)^3} G^T_{\alpha\alpha}(k + q, i\omega_n + iv_m) G^T_{\beta\beta}(k, i\omega_n) \tag{41}$$

The expressions of the two other components which are needed in Eq. (39), i.e., T^z_{----} and T^z_{-++-}, are obtained from those in Eq. (40) by interchanging $+$ and $-$. In Fig. 2a the diagrammatic representation of the T matrix in terms of the Abrikosov-type diagrams is resolved in terms of usual diagrams containing interaction lines: one obtains "ladders" and "strings of bubbles."

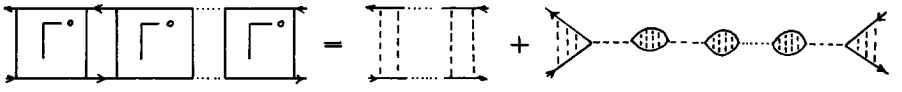
Second, the auxiliary field **H** is chosen to be directed along the x axis. In Fig. 2b the T matrix, given again by a chain of Γ^0's, is resolved in terms of usual diagrams. One recognizes by comparison of the right-hand sides of a and b in Fig. 2 that in the latter case one vertex in each bubble is dressed by a ladder of interaction lines. Again Eq. (38) for the T matrix can be solved by means of Fourier transformation. However, the solution of the system of linear algebraic equations for the 16 components $T^x_{\alpha\beta\gamma\delta}(q, iv_m)$ (the superscript x denotes that **H** is along the x axis) is much more tedious than that for the components T^z because now there are off-diagonal components of $G^T_{\alpha\beta}$ giving rise to many coefficients being different from zero. For brevity we omit the resulting expressions. In this way Johansson[8] has determined the poles of the components T^x.

One may test the covariance of the T matrix with respect to that rotation in spin space corresponding to a rotation of **H** from the z axis to the x axis. Then, the transformation matrix $\Theta_{\alpha\beta}$ (which can be obtained by integrating the infinitesimal rotation matrix $(\delta_{\alpha\beta} - i\Lambda_{\alpha\beta})$, introduced in Section 2) becomes:

$$\Theta_{\alpha\beta} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \qquad \Theta^{-1}_{\alpha\beta} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \tag{42}$$



(a)



(b)

Fig. 2. Schematic representation of the T matrix in terms of diagrams of the Abrikosov *et al.*[3] type (left-hand sides) and usual type (right-hand sides) for: (a) magnetization directed along the z axis (that is the axis of spin quantization), and (b) magnetization directed along the x axis. Solid lines represent matrix Green's functions $G^T_{\alpha\beta}$ (the spin indices at the ends of these lines have been omitted); in (a) it is diagonal, in (b) it has also off-diagonal components. A box means the undressed four-point vertex Γ^0 [Eq. (13)]. A dashed line represents the contact interaction acting only between particles having different spin direction.

In fact, one finds that the components T^x and T^z, determined from the corresponding systems of equations, are related by

$$T^x_{\alpha\beta\gamma\delta}(q, iv_m) = \Theta_{\alpha\mu}\Theta_{\beta\nu}T^z_{\mu\nu\zeta\eta}(q, iv_m)\Theta^{-1}_{\zeta\gamma}\Theta^{-1}_{\eta\delta} \tag{43}$$

From Eq. (43) it follows immediately that the poles of the components T^x are identical to those of the components T^z.

The "exchange splitting energy" is given by

$$\Sigma^{T^z}_{++} - \Sigma^{T^z}_{--} \quad \text{or} \quad 2\Sigma^{T^x}_{+-}$$

for **H** directed along the z axis and x axis, respectively. Inserting the expressions of T^z and G^{T^z} or T^x and G^{T^x}, respectively, into Eq. (39) one finds that the resulting two expressions for the exchange splitting energy are identical (the superscripts z and x on Σ^T and G^T denote, of course, the direction of **H**). Again this result is a consequence of the covariance of the particle–hole T-matrix approximation with respect to rotations of **H**; recall that this covariance property is guaranteed for any approximation constructed in accordance with the conditions 1, 2, and 3 of Section 2.

Equations (39)–(41), determining the self-energy part in the particle–hole T-matrix approximation, have been given previously by Brinkman and Engelsberg.[7] In their explicit evaluation of these equations they inserted, instead of the Green's function G^T containing just this self-energy part Σ^T, the Hartree–Fock Green's functions with energies $E^{\mathrm{HF}}_{\pm}$, given in Eq. (16), into Eqs. (39)–(41). They have shown that the resulting self-energy parts, denoted here by $\bar{\Sigma}_{\pm\pm}(k, \omega)$, have a large slope at $k = k_{\pm}$ with respect to ω at $\omega = 0$; this slope diverges like

ln M as M tends to zero (M is the relative magnetization). This singularity of $\bar{\Sigma}$ leads to divergencies in the effective mass and the specific heat. In order to illustrate the dependence of $\bar{\Sigma}_{\pm\pm}(k, \omega)$ on ω and M at $k = k_{\pm}$ several curves obtained by numerical calculations are shown in Fig. 3. In our numerical calculations only that part of $\bar{\Sigma}$ arising from the spin-wave part of T^z [second expression in Eq. (40) and that of $T^z{}_{-++-}$] has been taken into account; further, the temperature is taken to be zero and the Stoner equation [Eq. (19)] has been used to relate the magnetization and coupling constant $\bar{V}$.

In order to improve the evaluation of the Eqs. (39)–(41), given by Brinkman and Engelsberg[7] and shown in Fig. 3, we assumed that the main contributions to the integrals in Eqs. (39) and (41) arise from the immediate vicinities of the Fermi surfaces ($\omega = 0$, $k = k_{\pm}$; we consider here only the case of zero temperature). If this assumption is correct one may replace the self-energy parts Σ^T occurring in the G^T's by two constants that are the values of Σ^T at their respective Fermi

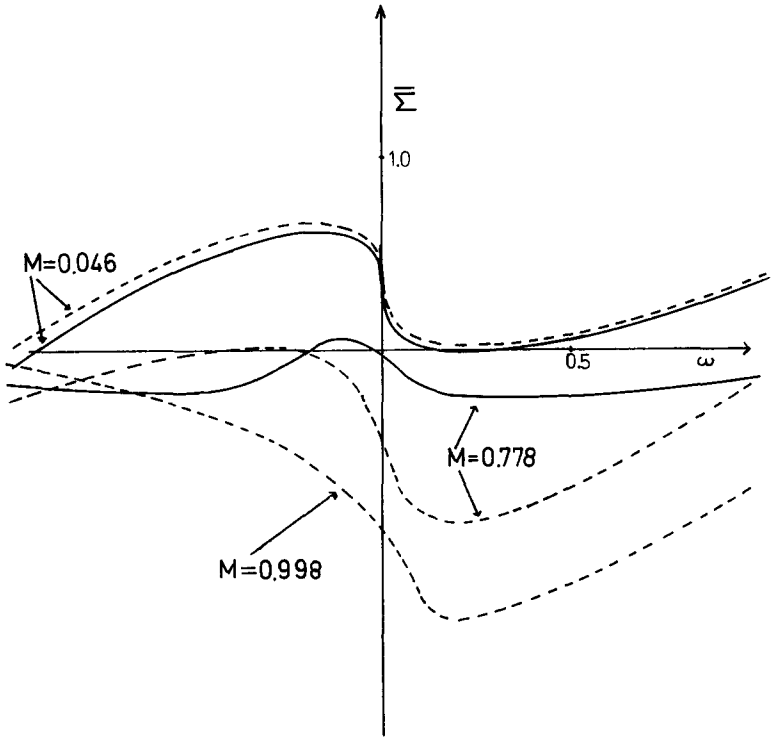


Fig. 3. Approximate self-energy parts at zero temperature, $\bar{\Sigma}_{\pm\pm}(k, \omega)$, plotted vs. ω for $k = k_{\pm}$ (Fermi sphere radii) and various values of the relative magnetization M. $\bar{\Sigma}$ and ω are measured in units $k_+^2/2m$. Solid lines: $\bar{\Sigma}_{++}$; dashed lines: $\bar{\Sigma}_{--}$. For $M = 0.998$ the curve of $\bar{\Sigma}_{++}$ is almost identical to the ω axis. These curves have been obtained numerically from the Eqs. (39)–(41), valid for the particle–hole T-matrix approximation, by approximating the G^T, s on the right-hand sides of these equations by the Hartree–Fock Green's functions and taking into account only the spin-wave part of the T matrix.

surfaces. These constants have to be determined self-consistently from Eqs. (39)–(41). Then the equilibrium conditions, i.e.,

$$\begin{aligned}(2m)^{-1}(k_+^2 - k_-^2) &= \Sigma^T_{--}(\omega = 0, k = k_-) - \Sigma^T_{++}(\omega = 0, k = k_+) \\ N/\Omega &= (6\pi^2)^{-1}(k_+^3 + k_-^3)\end{aligned} \tag{44}$$

gives a relation between the magnetization M and the coupling constant $\bar{V}$ corresponding to the Stoner equation (19). However, this procedure leads to a contradiction to the requirement of the analyticity of the $T^z(q, \nu)$ in the upper half of the complex ν plane. One finds for a given M a higher value of the corresponding $\bar{V}$ than that following from Eq. (19). In analogy to the investigations of the analyticity of the Hartree–Fock susceptibilities in Section 3 it follows that the $T_{\alpha\beta\gamma\delta}(q, \nu)$, approximated in the way described above, have poles in the upper half of the complex ν plane.

From this investigation one might draw the conclusion that any evaluation of the system of the T-matrix equations where the self-energy parts on the right-hand sides of these equations [Eqs. (39)–(41)] are replaced by constants, as was done, for instance, in Ref. 7, are suspect. Thus it seems to be necessary to solve the whole set of Eqs. (39)–(41) for the unknowns Σ^T, or G^T, and the T-matrix self-consistently.

The next step in the framework of the particle–hole T-matrix approximation scheme would be to calculate the correlation function, and thus the susceptibility. For this purpose one has to insert into the integral equation, Eq. (7), for L the corresponding approximation for the irreducible vertex part Γ^{1T}. This is given by the expression in Eq. (26) in Ref. 1 containing integrals of products of two T matrices. Of course, all G,s occurring in Eq. (7) and Eq. (26) in Ref. 1 become G^T,s. However, so far not even the Green's functions G^T and the T matrix have been calculated in a satisfactory way.

APPENDIX

In this appendix the existence of zeros of the denominators of the Hartree–Fock susceptibilities in Eqs. (22) and (23) is investigated. Performing the sum over $i\omega_n$ one obtains from Eq. (24)

$$\chi_{\alpha\beta}(q, i\nu_m) = \int \frac{d^3k}{(2\pi)^3} \frac{f[E_\alpha(k+q)] - f[E_\beta(k)]}{E_\beta(k) - E_\alpha(k+q) + i\nu_m} \tag{A1}$$

where f denotes the Fermi function. From Eq. (A1) one can easily derive the following properties of χ^0 with respect to its frequency variable (whenever possible the variable q is omitted):

$$\operatorname{Im}[\chi^0_{\alpha\beta}(\omega + i\delta)] \operatorname{sgn} \omega \geq 0 \qquad \chi_{\alpha\beta}(z) = \chi_{\beta\alpha}(-z) \tag{A2}$$

Further, one needs the following statements[10] for a function $g(z)$ having the property $g(z) = g(-z)$ and permitting a spectral representation, i.e.,

$$g(z) = 2\int_0^\infty \frac{d\omega'}{\pi}\,\frac{\omega' \operatorname{Im} g(\omega' + i\delta)}{\omega'^2 - z^2} \quad (\text{where } z = x + iy)$$
$$\operatorname{Im} g(z) = 4xy\int_0^\infty \frac{d\omega'}{\pi}\,\frac{\omega' \operatorname{Im} g(\omega' + i\delta)}{(\omega'^2 - x^2 - y^2)^2 + 4x^2y^2} \tag{A3}$$

These statements are: (a) if $\operatorname{Im}(g(x + i\delta))$ is positive or negative definite, $\operatorname{Im}(g(z))$ can vanish only on the real or imaginary axis of the complex z plane; (b) $\operatorname{Im}(g(z))$ does not change its sign within a quadrant of the complex z plane; and (c) $g(iy)$ has an extremum at $y = 0$.

First, the existence of poles of $\chi_{zz}(z)$ in the upper half of the complex z plane is examined; these poles would be given by the solutions of the following coupled equations:

$$1 - V^2 \operatorname{Re}\chi^0_{+\,+}(z) \operatorname{Re}\chi^0_{-\,-}(z) + V^2 \operatorname{Im}\chi^0_{+\,+}(z) \operatorname{Im}\chi^0_{-\,-}(z) = 0 \tag{A4}$$

$$\operatorname{Re}\chi^0_{+\,+}(z) \operatorname{Im}\chi^0_{-\,-}(z) + \operatorname{Re}\chi^0_{-\,-}(z) \operatorname{Im}\chi^0_{+\,+}(z) = 0 \tag{A5}$$

The function $\chi^0_{\alpha\alpha}(z)$ has the properties of $g(z)$ stated above. One may convince oneself that all possible solutions z_0 of Eqs. (A4) and (A5) have to satisfy the equations $\operatorname{Im}(\chi_{+\,+}(z_0)) = \operatorname{Im}(\chi_{-\,-}(z_0)) = 0$. So the investigation is confined to the imaginary axis. Otherwise one is led to a contradiction as can be seen by inserting Eq. (A5) into (A4) and using the definiteness (c) of $\operatorname{Im}(\chi_{\alpha\alpha}(z))$. Since $\chi_{\alpha\alpha}(iy)$ has a maximum at $y = 0$ a pole cannot occur in the upper half of the complex frequency plane if

$$V^2\chi_{+\,+}(q, 0)\chi_{-\,-}(q, 0) < 1 \tag{A6}$$

In the special case where $T = 0$ and $\varepsilon(k) = k^2/2m$ the quantity $\chi_{\alpha\beta}(q, 0)$ has a maximum at $q = 0$. Therefore the critical value of the coupling constant V_{cr} is given by

$$V_{cr}^2 \frac{m}{4\pi^2} k_+ k_- - 1 = 0 \tag{A7}$$

where we have used

$$\chi_{\pm\,\pm}(0, 0) = \frac{m}{2\pi^2} k_\pm$$

Taking into account the definitions given in Eqs. (17), (18), and (20), the relation in Eq. (27) can easily be derived.

Instead of examining the occurrence of poles in the transverse susceptibility [Eq. (22)] the zeros of an auxiliary function $[f(z)]^{-1}$ where

$$f(z) = \frac{1}{1 - V\chi_{+\,-}} + \frac{1}{1 - V\chi_{-\,+}} = \frac{2 - V(\chi_{+\,-} + \chi_{-\,+})}{(1 - V\chi_{+\,-})(1 - V\chi_{-\,+})} \tag{A8}$$

are investigated. Assuming at the beginning that $2 - V(\chi_{+-} + \chi_{-+}) \neq 0$ then $[f(z)]^{-1}$ has the properties of $g(z)$ stated above. Just as before one finds the condition $[f(0)]^{-1} > 0$ to be sufficient to exclude the possibility of poles in the upper half plane. Since this condition is equivalent to $f(0) > 0$ one finds with the help of the symmetry relation $\chi_{+-}(0) = \chi_{-+}(0)$ the critical value of V:

$$1 - V_{cr}\chi_{+-}(q, 0) = 0 \tag{A9}$$

The same condition ensures also that $(2 - V(\chi_{++} + \chi_{--})) \neq 0$. For the special case where $T = 0$ and $\varepsilon(k) = k^2/2m$ one sees with the help of the relation [from Eq. (16)]

$$E_+^{\mathrm{HF}}(k) - E_-^{\mathrm{HF}}(k) = \frac{k_-^2}{2m} - \frac{k_+^2}{2m}$$

that Eq. (A9) is equivalent to

$$\frac{k_+^2}{2m} - \frac{k_-^2}{2m} - \frac{V_{cr}}{6\pi^2}(k_+^3 - k_-^3) = 0 \tag{A10}$$

Inserting the definitions of Eqs. (17), (18), and (20) one obtains Eq. (19) (the Stoner equation) for V_{cr}.

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