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Green's function in a disordered spin-exchange field

H. Capellmann
Institut Laue-Langevin, B.P. 156, 38042 Grenoble, France *
and Institut of Theoretical Physik, TH Aachen, Germany

R. E. Prange
Department of Physics and Astronomy and Center for Theoretical Physics,
University of Maryland, College Park, Maryland 20742

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The temperature dependence of the single-electron Green's function of an itinerant ferromagnet has been recently studied by Korenman and Prange [Phys. Rev. Lett. 44, 1291 (1980)]. In addition to the general importance of the single-electron Green's function the study is of special interest because of the photoemission measurements of Eastman *et al.* [Phys. Rev. Lett. 40, 1514 (1978)], and the improved experiments of Gerhardt *et al.* (unpublished). Korenman and Prange obtained an unusual form for the Green's function, by an equation-of-motion decoupling technique (unpublished). The purpose of this note is to show that the identical form for the Green's function is obtained by two completely different methods, one based on the continued-fraction expansion, and the other based on an expansion and resummation method applied to the Green's function in the form found by Capellmann [J. Phys. F 4, 1466 (1974)]. The forms found are identical, and the precise expressions are in fact very close to that of Korenman and Prange. They differ because of some additional approximations made, primarily the neglect of the time dependence of the disorder. It is, however, clear that the form of the Green's function has a remarkable structure for the type of disorder envisaged.

I. INTRODUCTION

A study of the single electron Green's function is always of interest because of the fundamental nature of this object. It can, as well, be measured directly in angle-resolved photoemission experiments. Such experiments were recently performed[1,2] on the ferromagnetic $3d$ transition metals, which are itinerant. These experiments were of particular importance since they were the first direct measure of the exchange split band structure. The experiments in the case of nickel have been extended above the Curie temperature T_C. The results are consistent with the existence of a nonvanishing exchange splitting above T_C, although the resolution of the experiment is such that theoretical interpretation is required.

The notion of a nonvanishing exchange splitting above T_C is central to a number of theoretical approaches[3-5] to itinerant electron ferromagnetism. Moriya[6] has provided a recent review of this subject. According to these ideas, a typical magnetization configuration, although it may be time dependent, and without any net long time or long-range order, will still possess significant short-range order. Locally the average magnitude of the magnetization is not much different from that at the absolute zero of temperature. The fluctuations in the magnitude are fast, and similar to the ground-state fluctuations. The short-range magnetic order then allows a definition of "local bands" which are exchange split with respect to the local direction of magnetization. This preferred direction varies rather smoothly throughout the crystal. Its time variation is of lesser importance, and will be neglected in this paper.

Based on this picture, Korenman and Prange[7] recently used an equation of motion decoupling technique for the Green's function to discuss the temperature dependence and give a novel interpretation of the photoemission data.

Here we shall give two alternative methods which yield equivalent results. The Green's function is sought for the independent electron model with Hamiltonian

$$H=-\frac{\nabla^2}{2m}-\frac{\Delta}{2}\underline{\sigma}\cdot\vec{\mu}(\vec{r}) \quad . \qquad (1)$$

In this equation $\underline{\sigma}$ is the Pauli matrix, $\vec{\mu}$ is a unit vector which depends on the position variable $\vec{r}$, and Δ is a parameter, corresponding to the exchange splitting. The Hamiltonian need not have this simple parabolic form, which is chosen only for illustration. Indeed, we shall use a more general Hamiltonian in Sec. III. In principle, one must determine Δ self-consistently, according to the relation

$$\vec{\mu}\,\Delta=U\langle\vec{M}(\vec{r})\rangle \quad , \qquad (2)$$

with U the intra-atomic Coulomb repulsion. We shall

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not concern ourselves with this aspect of the problem, however, but simply consider the problem of finding the single electron Green's function for the Hamiltonian (1), averaged over appropriate configurations of the unit vector $\vec{\mu}(\vec{r})$.

The (inverse) Green's function is customarily written

$$1/G(k,E)=E-\epsilon_k-M(k,E) \quad , \tag{3}$$

where M is the self-energy operator and ϵ_k is in this case $k^2/2m$. Here we must be more precise and specify that we are speaking of the $\uparrow\uparrow$ component of G, as G is generally a matrix in the spin indices. We shall imagine for the moment, however, that we are considering configurations of exchange field directions which on the average vanish, corresponding to a temperature above the Curie point. Then G is proportional to the unit matrix in spin space. The result of Korenman and Prange is that $M(k,E)$ can be written

$$M(k,E)=\frac{\Delta^2}{4}\frac{1}{E-\epsilon_k-2\Sigma(k,E)} \quad . \tag{4}$$

Here Σ has a form which resembles a standard electron-magnon self-energy in a low approximation. We shall display Σ later.

This rather unusual form practically guarantees that G will have a multiple pole structure, and indeed that is exactly what is found. Korenman[8] has given an intuitive description of why this multiple pole structure is necessary physically. Briefly, it is needed so that the excitation of (collective) spin waves can be reflected in the structure of the single particle Green's function. The excitation of the spin waves must of course lower the net magnetization, and at the same time, at long wavelengths, cannot change the electronic energy.[5] It does this by introducing into the spin-up Green's function an extra pole corresponding to a spin-down electron, and at the same time the residue at the up-spin pole is reduced.

In the next section, we shall derive this form, and an approximation to Σ, by the method of continued fractions. In Sec. III, we shall carry out the derivation by a method based on series resummation.

II. CONTINUED FRACTION EXPANSION

The method of continued fractions has most vigorously been exploited recently by the Cambridge group.[9] In that method, one chooses to find the Green's function, defined by the formula,

$$G(k,E)=\left\langle 0\left|\frac{1}{E-H}\right|0\right\rangle \quad , \tag{5}$$

where the state $|0\rangle$ is in general arbitrary. For the case at hand, where we wish to find the Green's function for a definite momentum, it is

$$|0\rangle=(1/\sqrt{V})e^{i\vec{k}\cdot\vec{r}}\begin{bmatrix}1\\0\end{bmatrix} \quad . \tag{6}$$

Here V is the total volume of the system.

Here, it is enough to find the Green's function for a typical configuration, as this is equivalent to a spatial average, which will be identical to the result of an ensemble average.

The continued fraction method sets up a linear chain or heirarchy of states $|N\rangle$ according to the recursion relations

$$\begin{aligned} H|0\rangle &= a_0|0\rangle+b_1|1\rangle \quad , \\ H|N\rangle &= b_N^*|N-1\rangle+a_N|N\rangle+b_{N+1}|N+1\rangle \\ &\qquad\qquad (N>0) \quad . \end{aligned} \tag{7}$$

The coefficients a_N and b_N as well as the states can readily be found by using the orthonormality of the states. Having found the coefficients, the Green's function is expressed in continued fraction form by

$$G(k,E)=\cfrac{1}{E-a_0-\cfrac{|b_1|^2}{E-a_1-\cfrac{|b_2|^2}{E-a_2\cdots}}} \quad . \tag{8}$$

It is easily found that

$$a_0=\epsilon_k,\ \ b_1=\Delta/2,\ \ |1\rangle=-\underline{\sigma}\cdot\vec{\mu}(\vec{r})|0\rangle \quad ,$$

$$a_1=\langle 1|H|1\rangle=\epsilon_k+2\langle a^2\rangle/m \quad ,$$

with $\langle a^2\rangle$ the measure of short-range order introduced by Korenman, Murray, and Prange,[5] namely,

$$\langle a^2\rangle=\langle(\nabla\vec{\mu})^2\rangle/4 \quad .$$

The brackets indicate spatial (or ensemble) averages. So far, all is exact, provided the space average $\vec{\mu}$ vanishes. One may also get precisely the same results below T_C by considering the spin trace of the Green's function, but in that case it is necessary to introduce projection operators rather than states, as Mori[10] has done.

It is straightforward, although increasingly tedious, to write down the coefficients to any desired order. Accordingly, we make now the approximation that $\langle a^2\rangle$ is small, and keep only the leading terms in the remainder of the expansion. This, while not quite adequate numerically for nickel, will give at least the main form of the result. The approximation of small $\langle a^2\rangle$ is the short-range magnetic order approximation of Capellmann,[3] and of Korenman, Murray, and Prange, who have discussed its validity and experimental justification.

We therefore shall keep b_2 to first order (the leading order) in $\nabla\vec{\mu}$, and all the remaining terms to zeroth order in this quantity. We find

$$b_2|2\rangle \approx (-i/m)(\vec{\mathrm{k}}\cdot\nabla)(\vec{\mu}\cdot\underline{\sigma})|0\rangle \ , \quad |b_2|^2 = \langle|\vec{\mathrm{k}}\cdot\nabla\vec{\mu}|^2\rangle/m^2 = \langle|\vec{\mathrm{v}}_k\cdot\nabla\vec{\mu}|^2\rangle \ , \quad a_3 \approx a_4 \approx \epsilon_k ,$$

$$b_3 \approx \Delta/2 \ , \quad b_4 \approx 0 \ .$$

The result for M is thus

$$M(k,E) = \frac{\Delta^2}{4}\,\frac{1}{E-\epsilon_k-\langle(\vec{\nabla}\cdot\vec{\mu})^2\rangle/2m-\dfrac{\langle(\vec{\mathrm{v}}\cdot\nabla\vec{\mu})^2\rangle}{E-\epsilon_k-\dfrac{(\Delta/2)^2}{E-\epsilon_k}}} \ . \tag{9}$$

The expression for Σ is therefore

$$2\Sigma(k,E) = \langle(\vec{\nabla}\cdot\vec{\mu})^2\rangle/2m - \frac{\langle(\vec{\mathrm{v}}\cdot\vec{\nabla}\mu)^2\rangle}{E-\epsilon_k-\dfrac{(\Delta/2)^2}{E-\epsilon_k}} \ .$$

which can be written as

$$\Sigma(k,E) = 2\langle a^2\rangle/2m - \langle|\vec{\mathrm{v}}\cdot\nabla\vec{\mu}|^2\rangle[(E-\epsilon_k-\Delta/2)^{-1}+(E-\epsilon_k+\Delta/2)^{-1}] \ .$$

This displays the character of Σ as the sum of "elementary" self-energies, one for spin-up electrons and one for spin down. This self-energy is discussed further in Ref. 11.

The result, Eq. (9), is identical to that of Koreman and Prange, to the order here maintained, and with the neglect of the time dependence of $\vec{\mu}$.

III. SERIES RESUMMATION

In this section we use the Green's function technique derived previously by one of us[3] for itinerant ferromagnetism in the $3d$-transition metals. This technique proceeds as follows: The definition of the Green's function

$$g_{is,js'}(\kappa,t) = -i\langle\kappa|T[c_{is}(t)c^{\dagger}_{js'}(0)]|\kappa\rangle \tag{10}$$

is used where $|\kappa\rangle$ is some typical configuration (i.e., some vector of Hilbert space which is important in the thermal averages to be carried out later). Here t is a time variable, T is the usual time ordering operator, and $c_{is}(c^{\dagger}_{is})$ are annihilation (creation) operators in a local site representation, with i the site index, and s the spin index. The matrix function g is calculated using a Hamiltonian in which the interaction term is replaced by molecular fields (exchange fields) which are determined self-consistently for each $|\kappa\rangle$ according to Eq. (2). This Hamiltonian is thus

$$H = t_{ij}\delta_{ss'} - \tfrac{1}{2}\Delta\vec{\mu}_i\,\underline{\sigma}_{ss'}\delta_{ij} \equiv (H_0+M)_{is,js'} \ . \tag{11}$$

Since this is a single-particle Hamiltonian, we can drop the creation and annihilation operators and deal directly with the Hamiltonian matrix. This single-particle Hamiltonian is identical to that of Eq. (1) except that a discrete site representation has been used and the kinetic and spin independent potential-energy terms are represented by a "tight-binding" hopping matrix, t, which transfers an electron from site j to site i. The representation, Eq. (11), is thus somewhat more general than that of Eq. (1). It is necessary to generalize still further (to multiple bands) in order to have a Hamiltonian capable of representing iron or nickel accurately.

Next, the appropriate thermal averages are carried out to determine the thermal properties. The time Fourier transformed (and configuration dependent) Green's function, in a matrix notation, is written as

$$g = \frac{1}{E-H_0-M} \ . \tag{12}$$

The configuration dependence is contained in the exchange field direction $\vec{\mu}_i$, which for the most important configurations are not translationally invariant, but do have short-range magnetic order. This aspect may be exploited by using an expansion in the commutator in the following way. Let

$$K = [H_0, M] \ . \tag{13}$$

One can then show[3] that g may be written as

$$g = (P^+g^+ + P^-g^-)\frac{1}{1-Kg^+g^-} \ . \tag{14}$$

The $P^{\pm}$ are projection operator matrices onto the local direction of the magnetization and the $g^{\pm}$ are Green's functions for spin up or down electrons. The quantization axis is the *local* direction of the magnetization

$$P^{\pm} = \delta_{ij}(\underline{1} \pm \vec{\mu}_i \cdot \underline{\sigma})/2 \ , \qquad g^{\pm} = \frac{1}{E - H_0 \mp \Delta/2} \ . \tag{15}$$

Here, $\underline{1}$ is the unit matrix in spin space.

We are interested in a configurational average (denoted by angular brackets $\langle \ \rangle$) of the spin trace of g, which we shall call $G = \langle \mathrm{Tr} g \rangle$. Because of the spin trace (or the configuration average, above T_C) only even powers of $\vec{\mu}$ will survive this average. We can expand g in powers of K, throw away all odd powers in $\underline{\mu}$, and resum. It follows that

$$G = \left\langle [(g^+ + g^-)/2 + A_2 g^+ g^-] \frac{1}{1 - A_1 g^+ g^-} \right\rangle \ , \tag{16}$$

where the A_i are given by

$$A_1 = K g^+ g^- K \ , \tag{17}$$

$$A_2 = M g^+ g^- K \ . \tag{18}$$

Equation (16) is exact. At this point we make the simplest possible approximation and replace the quantities A_i by their configurational averages $\langle A_i \rangle$. This yields G in terms of the correlation function Γ_{ij}, defined as

$$\Gamma_{ij} = \langle \vec{\mu}_i \cdot \vec{\mu}_j \rangle \ . \tag{19}$$

G can be written in the form given by Eqs. (3) and (4), with

$$2\Sigma = \left[-\langle A_2 \rangle + \frac{E - H_0}{\Delta^2/4} \langle A_1 \rangle + \frac{(E - H_0)^2}{\Delta^2/4} \langle A_2 \rangle \right] \Bigg/ \left[1 + \frac{\langle A_1 \rangle}{\Delta^2/4} + \frac{\langle A_2 \rangle (E - H_0)}{\Delta_2/4} \right] \ . \tag{20}$$

The result of Ref. 7 is recovered if the $\langle A_i \rangle$ in the denominator of Σ are neglected. Using the Fourier-transformed quantities

$$H_0 \to \epsilon_k, \quad \Gamma_{ij} \to \Gamma_k; \quad \Sigma_{ij} \to \Sigma_k \ ,$$

we obtain

$$2\Sigma_k \cong -\sum_q \Gamma_q \left[(\epsilon_k - \epsilon_{k-q}) - \frac{(E - \epsilon_{k-q})(\epsilon_k - \epsilon_{k-q})}{(E - \epsilon_{k-q})^2 - \Delta^2/4} \right] \ . \tag{21}$$

IV. DISCUSSION

According to the continued fraction expansion of Sec. II, the form of the Green's function for a Hamiltonian of the type considered is rather special. It might be thought that this form is a tautology, and that any self-energy could be cast into the structure found. This is not true, because the structure determines the *large energy behavior* or alternatively, the *first moments of the density of states* of the Green's function.

There are of course other approximations in common use in the theory of disordered systems. Most notable is the single-site coherent potential approximation (CPA). The CPA is the simplest single-site approximation, based on complete disorder with no short-range order, which has the structure of Eq. (3). The "average potential," and "average t-matrix" approximations do not have this structure, for example. (To be precise, in the CPA, M is independent of k, as is Σ, and the explicit ϵ_k is replaced by its average. The quantity M in the CPA is the single-site coherent potential of the effective medium.) It has long been felt that for many applications the CPA is the best approximation available.

What this paper has shown is that there is an approximation with similar virtues available for the case of short-range order, and that this approximation is essentially unique, although it can be derived in a number of ways.

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[*] Present address.

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