Condition for spin-rotational invariance in a semi-infinite itinerant-electron ferromagnet

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The dynamic transverse spin susceptibility χ_{+-} of a tight-binding Hubbard model of an itinerant-electron ferromagnet must exhibit a zero-frequency spin-wave mode if the starting Hamiltonian is spin-rotationally invariant. We give an explicit proof that χ_{+-} for a semi-infinite Hubbard model will indeed have such a Goldstone mode if it is computed with the self-consistent-field approximation. We also derive a necessary and sufficient condition on the free-particle susceptibility χ^0_{+-} which ensures that χ_{+-} computed in this approximation will be spin-rotational invariant. Our work complements the more formal results of Brandt and co-workers on conserving approximations. We use our sum rule for χ^0_{+-} to discuss various simplified models which have been used to describe the effect of a planar surface in Hubbard models. In particular, the work of Mathon is discussed.

I. INTRODUCTION

In the theory of ferromagnetism, the close relationship between the breaking of rotational spin invariance of the original Hamiltonian and the appearance of a zero-frequency spin-wave resonance in the dynamic transverse spin response function is well understood (see, for example, p. 676 of Ref. 1). The original symmetry in spin space is destroyed by spontaneous ordering along some direction (described by the appearance of a static exchange field) but is dynamically restored by the exchange interaction through the appearance of a low-frequency Goldstone mode. This makes it clear that one must treat the static and dynamic exchange fields at the *same* level of approximation.

In the present paper, we discuss this problem within the context of a tight-binding model of an itinerant-electron ferromagnet with a planar boundary.[1,2] We give an *explicit* proof that the transverse spin response function χ_{+-} does indeed have a zero-frequency pole if it is calculated within the self-consistent-field approximation (SCF) [sometimes called the random-phase approximation (RPA)]. In particular, we show that this will result *if* the free-particle response function χ^0_{+-} is evaluated in terms of the eigenstates of the static SCF Hamiltonian. This is not unexpected in view of the work of Brandt and co-workers.[3,4] Generalizing the method of Baym and Kadanoff[5] to construct spin conserving approximations for χ_{+-} from a given self-energy, Brandt, Lustfield, Pesch, and Tewordt[4] proved that the Hartree-Fock and the particle-hole T-matrix approximations give response functions which are manifestly spin-rotational invariant and hence exhibit the $\omega=0$ Goldstone mode.

The advantage of our approach is that it requires little formalism and, as a by-product, leads to a sum rule on χ^0_{+-} which must be satisfied if $\chi^{\rm SCF}_{+-}$ is to exhibit the $\omega=0$ pole. This sum rule may be quite useful in conjunction with approximate solutions of the SCF integral equation for χ_{+-}, based on a calculation of χ^0_{+-} using a realistic electronic band structure. This is important since, in contrast with localized spin models,[6] calculation of the spin-wave modes in bounded itinerant-electron models[1,2] is quite complicated and it is easy to lose spin-rotational invariance. The classical infinite-barrier model (CIBM) approximation for χ^0_{+-} used by Gumbs and Griffin[1] (GG) does not satisfy this sum rule and hence it leads to a χ_{+-} which does not satisfy spin-rotational invariance (because it ignores changes in the surface magnetization). However, we show that their result $\chi^{0\rm G}_{+-}$ is still useful since the full SCF integral equation can be reformulated in terms of $\chi^{0\rm G}_{+-}$, with only the surface changes left as a perturbation. This means that $\chi^{0\rm G}_{+-}$ is, in fact, an appropriate input response function in the approach recently suggested by Mathon[2] for solving the SCF integral equation for χ_{+-}.

We remark that a similar analysis can be given for the SCF dynamic response function of systems with other kinds of broken symmetry.

II. CRITERION FOR SPIN-ROTATIONAL INVARIANCE

We work with the standard tight-binding model of an itinerant-electron ferromagnet. We refer to Ref. 1 for notation and further discussion of this model. Restricting ourselves to on-site matrix elements for simplicity, the two-particle interaction reduces to [see Eq. (2.4) of GG]

$$\hat{V}=\tfrac{1}{2}\sum_l U(l)\hat{n}(l)\hat{n}(l)-\sum_l I(l)\mathbf{s}(l)\cdot\mathbf{s}(l) \;, \tag{1}$$

where l represents sites and

$$\hat{s}_+(l)=\hat{c}^\dagger_{l\uparrow}\hat{c}_{l\downarrow}\;,\;\; \hat{s}_-(l)=\hat{c}^\dagger_{l\downarrow}\hat{c}_{l\uparrow}\;,$$
$$\hat{s}_z(l)=\tfrac{1}{2}(\hat{c}^\dagger_{l\uparrow}\hat{c}_{l\uparrow}-\hat{c}^\dagger_{l\downarrow}\hat{c}_{l\downarrow})\;. \tag{2}$$

As discussed in GG, the self-consistent-field approximation for (1) leads to

$$\chi_{+-}(l,l') \equiv i\int_{-\infty}^{\infty} dt e^{i\omega t}\langle[\hat{s}_+(l,t),\hat{s}_-(l',0)]\rangle\theta(t)$$
$$= \chi^0_{+-}(l,l') + \sum_{l_1}\chi^0_{+-}(l,l_1)I(l_1)\chi_{+-}(l_1,l') \ . \tag{3}$$

Here the free-electron transverse response function χ^0_{+-} is evaluated using the single-particle static SCF Hamiltonian

$$\hat{H}_{\rm SCF} = \sum_{l,l',\sigma} T_{ll'}\hat{c}^\dagger_{l\sigma}\hat{c}_{l'\sigma} + \sum_l V(l)\hat{n}(l) - \sum_l H_z(l)\hat{s}_z(l) \ , \tag{4}$$

where the effective fields are defined by

$$V(l) \equiv U(l)\langle\hat{n}(l)\rangle \ , \quad H_z(l) \equiv 2I(l)\langle\hat{s}_z(l)\rangle \ . \tag{5}$$

It is to be emphasized that $\hat{H}_{\rm SCF}$ is manifestly *not* spin-rotationally invariant.

The solution of (3) is very difficult even for the simple semi-infinite model GG discussed (simulated by setting all hopping integrals $T_{ll'}$ to zero between the planes $l=0$ and $l=a$ in a simple cubium model). However, we shall give an explicit proof that the solution of (3) is indeed consistent with the exact spin-rotational sum rule [see Eq. (2.20) of GG]

$$\sum_{l'}\chi_{+-}(l,l';\omega+i0^+) = -\frac{2\langle\hat{s}_z(l)\rangle}{\omega+i0^+} \ , \tag{6}$$

if $\chi^0_{+-}(l,l')$ is computed using (4). We recall that (6) is a direct consequence of the fact that the *total* spin operators

$$\hat{S}_\pm = \sum_l \hat{s}_\pm(l)$$

commute with (1).

To begin, we note that using (4), one may easily show that the equation of motion for $\hat{S}_-(t)$ only depends on the third term in (4), with

$$\frac{d\hat{S}_-(t)}{dt} = i[\hat{H}_{\rm SCF},\hat{S}_-(t)]$$
$$= i\sum_{l'}2I(l')\langle\hat{s}_z(l')\rangle\hat{s}_-(l',t) \ . \tag{7}$$

Taking the time derivative of $\chi^0_{+-}(l,l';t)$ as defined in the first line of (3) and using (7), one immediately finds

$$\omega\sum_{l'}\chi^0_{+-}(l,l';\omega) = \sum_{l'}\chi^0_{+-}(l,l';\omega)2I(l')$$
$$\times\langle\hat{s}_z(l')\rangle - 2\langle\hat{s}_z(l)\rangle \ . \tag{8}$$

This relation is a sum rule for $\chi^0_{+-}(l,l';\omega)$. We have shown that if χ^0_{+-} and $\langle\hat{s}_z(l)\rangle$ are computed in the SCF approximation given by (4), they must satisfy (8).

Going back to the SCF integral equation in (3), we sum over l' to give

$$\sum_{l'}\chi_{+-}(l,l') = \sum_{l'}\chi^0_{+-}(l,l')$$
$$+\sum_{l',l''}\chi^0_{+-}(l,l'')I(l'')\chi_{+-}(l'',l') \ . \tag{9}$$

Inserting (6) into (9) leads precisely to the requirement that χ^0_{+-} satisfy (8). Thus we see that (8) is a necessary consequence of the spin-rotational invariance sum rule (6). The remaining question is whether the validity of (8) is sufficient to guarantee (6). Using (8) in (9), we obtain after some rearranging

$$A(l) = \sum_{l'}\chi^0_{+-}(l,l',\omega)I(l')A(l') \ , \tag{10}$$

where we have defined the new function

$$A(l) \equiv \sum_{l'}\chi_{+-}(l,l';\omega) + \frac{2}{\omega}\langle\hat{s}_z(l)\rangle \ . \tag{11}$$

Clearly (10) may be viewed as a homogeneous system of linear algebraic equations for the variables $A(l)$. There may be nontrivial solutions of (10) for certain isolated values of ω. Apart from these values, the only possible solution of (10) is the trivial one, $A(l)=0$ for all l. Since $A(l)=0$ is equivalent to the sum rule (6), we see that (8) is sufficient to guarantee that (6) is valid, apart from isolated values of ω such that (10) has nontrivial solutions. With this proviso, we have proven that a necessary and sufficient condition that the full transverse spin response function $\chi_{+-}(l,l';\omega)$ given by the SCF equation (3) will exhibit a Goldstone zero-frequency pole [i.e., will satisfy the sum rule (6)] is that $\chi^0_{+-}(l,l';\omega)$ and $\langle\hat{s}_z(l)\rangle$ satisfy (8). This condition should be satisfied in any solution of (3), numerical or otherwise.

For *infinite* periodic systems, of course, (8) is trivial to satisfy since $I(l)=I_0$ and $\langle\hat{s}_z(l)\rangle=\bar{s}_B$, independent of the site l. In that case, (8) reduces to

$$\chi^0_{+-}(\mathbf{q}=\mathbf{0},\omega) \equiv \sum_{l'}\chi^0_{+-}(l,l';\omega) = \frac{-2\bar{s}_B}{\omega-2I_0\bar{s}_B} \ . \tag{12}$$

Thus the condition (8) simply leads to $\chi^0_{+-}(\mathbf{q}=\mathbf{0},\omega)$ having poles at the Stoner excitations. These ensure that the solution of (3) exhibits the required zero frequency pole

$$\chi_{+-}(\mathbf{q}=\mathbf{0},\omega) = \frac{\chi^0_{+-}(\mathbf{q}=\mathbf{0},\omega)}{1-I_0\chi^0_{+-}(\mathbf{q}=\mathbf{0},\omega)} = -\frac{2\bar{s}_B}{\omega} \ . \tag{13}$$

This example shows how the high-frequency Stoner excitations of χ^0_{+-} associated with the broken rotational symmetry are removed by the effect of the time-dependent symmetry-restoring exchange field.[1] In the case of semi-infinite systems, where $\langle\hat{s}_z(l)\rangle$ will be site-dependent near the boundary, the same physics is involved in (8) but it is not as transparent.

III. APPLICATIONS OF SUM RULE

In Sec. II, we have shown explicitly that the SCF approximation does in fact lead to the sum rule (8). Of course, other approximations for χ^0_{+-} may also be consistent with (8). In this section, we use (8) as a way of constructing and discussing models which will be spin-rotationally invariant.

The required sum rule (8) immediately shows the difficulty with the classical infinite barrier model (CIBM) approximation used by GG in an attempt to solve (3) for an itinerant-electron ferromagnet with a planar boundary. Assuming for simplicity translational symmetry in the x-y plane parallel to the surface, we Fourier transform (3) with respect $l_\parallel$-$l'_\parallel$ to give[1]

$$\chi_{+-}(l_z,l'_z;\mathbf{q}_\parallel,\omega)=\chi^0_{+-}(l_z,l';\mathbf{q}_\parallel,\omega)+\sum_{l''_z}\chi^0_{+-}(l_z,l''_z;\mathbf{q}_\parallel,\omega)I(l''_z)\chi_{+-}(l''_z,l'_z;\mathbf{q}_\parallel,\omega)\ . \quad (14)$$

Similarly, (8) is equivalent to

$$\sum_{l'_z}\chi^0_{+-}(l_z,l'_z;\mathbf{q}_\parallel=\mathbf{0},\omega)=\frac{2}{\omega}\sum_{l'_z}\chi^0_{+-}(l_z,l'_z;\mathbf{q}_\parallel=\mathbf{0},\omega)I(l'_z)\langle\hat{s}_z(l'_z)\rangle-\frac{2\langle\hat{s}_z(l_z)\rangle}{\omega}\ . \quad (15)$$

GG kept the geometrical effect of the planar boundary (classical reflection of electrons) but ignored surface-induced changes in both $I(l_z)$ and $\langle\hat{s}_z(l_z)\rangle$. The neglect of these surface-induced changes means that (15) reduces to

$$\sum_{l'_z}\chi^0_{+-}(l_z,l'_z;\mathbf{q}_\parallel=\mathbf{0},\omega)=\frac{-2\bar{s}_B}{\omega-2I_0\bar{s}_B}\ . \quad (16)$$

On the other hand, the CIBM approximation[1] for $\chi^0_{+-}(l_z,l'_z;\mathbf{q}_\parallel=\mathbf{0},\omega)$ is given by

$$\chi^0_{\rm cl}(l_z,l'_z)=\chi^{0B}_{+-}(l_z-l'_z)+\chi^{0B}_{+-}(l_z+l'_z)\ , \quad (17)$$

and this is not consistent with (16). Thus it is no surprise[1,2] that $\chi_{+-}(l_z,l'_z;\mathbf{q}_\parallel,\omega)$ does not satisfy (6).

In a more realistic model for the single-particle Green's function for a half-space,[1] $I(l)$ is assumed unchanged but the surface layer spin $\langle\hat{s}_z(l_z=a)\rangle=\bar{s}_S$ is assumed to be different from all the other (bulk) layers, $\langle\hat{s}_z(l_z\geq 2a)\rangle=\bar{s}_B$. For $\chi^0_{+-}(l_z,l'_z;\mathbf{q}_\parallel,\omega)$, we also assume that it is so short-ranged that it vanishes unless $l_z=l'_z$. In this case the solution of (14) is trivially obtained:

$$\chi_{+-}(l_z,l'_z;\mathbf{q}_\parallel,\omega)=\frac{\chi^0_{+-}(l_z,l_z;\mathbf{q}_\parallel,\omega)\delta_{l_z l'_z}}{1-I_0\chi^0_{+-}(l_z,l_z;\mathbf{q}_\parallel,\omega)}\ . \quad (18)$$

For the sum rule (15) to be satisfied, one may verify that for this microscopic model, we must have

$$\chi^0_{+-}(l_z,l_z;\mathbf{q}_\parallel=\mathbf{0},\omega)=\frac{-2\bar{s}_S}{\omega-2I_0\bar{s}_S},\ \text{for } l_z=a$$
$$=\frac{-2\bar{s}_B}{\omega-2I_0\bar{s}_B},\ \text{for } l_z=2a,3a,\ldots\ . \quad (19)$$

One sees explicitly that with (19), (18) is indeed consistent with the sum rule (6) in so far as

$$\chi_{+-}(l_z,l_z;\mathbf{q}_\parallel=\mathbf{0},\omega)=-2\langle\hat{s}_z(l_z)\rangle/\omega\ , \quad (20)$$

as required in this simple model.

In earlier work, Mathon[7] tried to improve upon GG by constructing a solvable model in which spin-rotational invariance could be ensured. He assumed $\langle\hat{s}_z(l)\rangle=\bar{s}_B$ for all layers but

$$I(l)=I_0+\Delta I,\ l_z=a\ ,$$
$$=I_0,\ l_z=2a,3a,\ldots\ , \quad (21)$$

and

$$\chi^0_{+-}(l_z,l'_z)=\chi^{0B}_{+-}(l_z-l'_z)+\Lambda\delta_{l,a}\delta_{l',a}\ . \quad (22)$$

Thus any effect due to reflection by the boundary is ignored [such as included in (17)] but a surface layer change is included. After a little calculation, one may verify that for this model, our sum rule (15) implies that

$$\Lambda(\mathbf{q}_\parallel,\omega)=\frac{2\bar{s}_B\Delta I}{\omega-2(I_0+\Delta I)\bar{s}_B}\chi^{0B}_{+-}(l_z=0;\mathbf{q}_\parallel,\omega)\ , \quad (23)$$

and

$$\chi^{0B}_{+-}(l_z\neq 0;\mathbf{q}_\parallel,\omega)=0\ . \quad (24)$$

In deriving these results, crucial use is made of the fact that $\chi^{0B}_{+-}(l_z-l'_z)$ satisfies (16). Since

$$\chi^{0B}_{+-}(q_z=0)=\sum_{l_z}\chi^{0B}_{+-}(l_z)=\chi^{0B}_{+-}(l_z=0)\ , \quad (25)$$

the last equality following from (24), and we know from (13) that to have a zero-frequency bulk spin-wave mode we must have

$$\lim_{\omega\to 0}\chi^{0B}_{+-}(\mathbf{q}=\mathbf{0},\omega)=\frac{1}{I_0}\ , \quad (26)$$

one can show that (23) reduces to

$$\lim_{\omega\to 0}\Lambda(\mathbf{q}_\parallel=\mathbf{0},\omega)=\frac{-\Delta I}{I_0(I_0+\Delta I)}\ . \quad (27)$$

This is Mathon's self-consistency condition for this model.[7] However, he did not obtain the additional requirement given by (24). The complete neglect of any reflection[8] and the extreme short-range of the correlations implied by (24) means that this cannot be taken as a realistic model for the surface of an itinerant-electron ferromagnet. The same point has been made by Mathon in his more recent work.[2]

Recently, Mathon[2] has discussed a way of solving (14) by analogy with methods developed for semi-infinite Heisenberg ferromagnets.[6] In this context, it is useful to separate $\chi^0_{+-}(l_z,l'_z)$ into the part $\chi^0_{\rm cl}(l_z,l'_z)$ corresponding to *classical* reflection of electrons at planar boundary given by (17) and a part $\chi^0_S(l_z,l'_z)$ which describes the effect of the surface-induced changes (localized at the first few atomic layers). Following Mathon,[2] one may define the "spin-wave" Green's function

$$\hat{\Gamma}\equiv(1-I_0\hat{\chi}^0_{+-})^{-1}=\hat{I}+I_0\hat{\chi}_{+-}\ , \quad (28)$$

where the matrix elements are labeled by the atomic planes parallel to boundary. One may then easily show that (14) can be written in the form

$$\hat{\Gamma}=\hat{\Gamma}_{\rm cl}+\hat{\Gamma}_{\rm cl}\hat{W}_S\hat{\Gamma}\ , \quad (29)$$

where

$$\hat{\Gamma}_{\rm cl}\equiv(\hat{I}-I_0\hat{\chi}^0_{\rm cl})^{-1}=\hat{I}+I_0\hat{\chi}_{\rm cl}\ , \quad (30)$$

and the surface perturbation is defined by

$$\hat{W}_S \equiv I_0(\hat{\chi}^0_{+-} - \hat{\chi}^0_{\rm cl}) = I_0\hat{\chi}^0_S \ . \tag{31}$$

The spin waves of the semi-infinite itinerant-electron ferromagnet are then given by the solutions of

$$\det|\hat{I} - \hat{\Gamma}_{\rm cl}\hat{W}_S| = 0 \ , \tag{32}$$

where $\hat{\Gamma}_{\rm cl}$ is the resolvent operator (30) associated with the CIBM response function $\hat{\chi}_{\rm cl}$ worked out by GG.

In terms of this formulation, GG's work consisted of approximating[9] $\hat{\Gamma}$ by $\hat{\Gamma}_{\rm cl}$, completely ignoring $\hat{W}_S$. As Mathon[2] has emphasized, however, it is crucial to include $\hat{W}_S$ and solve (29) self-consistently if spin-rotational invariance is to be obeyed. On the other hand, we see that $\hat{\Gamma}_{\rm cl}$ is the natural input in the sort of analysis given in Ref. 2. The *exact* solution of (14) using (17) is given by (3.40) of GG. After some calculation, this can be written in the equivalent form

$$\chi_{\rm cl}(l_z,l_z';\mathbf{q}_\parallel,\omega) = \chi^B_{\rm cl}(l_z,l_z') - \frac{1}{2I_0}\frac{1}{D}F(l_z)F(l_z') \ , \tag{33}$$

where [compare with (17)]

$$\chi^B_{\rm cl}(l_z,l_z') = \chi^B_{+-}(l_z - l_z';\mathbf{q}_\parallel,\omega) + \chi^B_{+-}(l_z + l_z';\mathbf{q}_\parallel,\omega) \ . \tag{34}$$

Here $\chi^B_{+-}(l_z - l_z')$ is the spin response function of an infinite tight-binding model as discussed in Refs. 1 and 2. In addition, we have introduced the functions

$$D(\mathbf{q}_\parallel,\omega) \equiv \frac{1}{N_0}\sum_{q_z}\frac{1}{\epsilon_M(q_z)} \ ,$$
$$F(l_z) \equiv \frac{2}{N_0}\sum_{q_z}\frac{\cos q_z l_z}{\epsilon_M(q_z)} \ , \tag{35}$$

where $\epsilon_M(q_z) \equiv 1 - I_0\chi^B_{+-}(\mathbf{q},\omega)$. As proven by GG, the poles of $\chi_{\rm cl}(l_z,l_z')$ in (33) are given by the zeros of D, not by the zeros of ϵ_M.

In our preceding discussion, we have argued that the most natural way of solving for the spin-wave Green's function $\hat{\Gamma}$ was to first split off the "classical reflection" or CIBM part of $\chi^0_{+-}(l_z,l_z')$ and treat the rest as a localized surface perturbation $\hat{W}$. However, the decomposition of χ^0_{+-} is somewhat arbitrary and other choices are possible. In fact, Mathon[2] separates out what he calls the "geometric approximation" to χ^0_{+-}. In contrast to the classical-reflection approximation given by (17) (which results from cutting electronic hopping matrix elements between the $l_z = a$ plane and the $l_z = 0$ plane), the geometric approximation is *defined* directly in terms of setting χ^0_{+-} equal to zero across the surface,[9] i.e.,

$$\chi^0_{+-}(l_z,l_z') = \chi^{0B}_{+-}(|l_z - l_z'|) - \delta_{la}\delta_{l'0}\chi^{0B}_{+-}(a) - \delta_{l0}\delta_{l'a}\chi^{0B}_{+-}(a) \ . \tag{36}$$

In contrast to (17), this gives a free-particle spin susceptibility which is identical to the bulk value for $l_z, l_z' \leq 0$ or $l_z, l_z' \geq a$. In particular, the reflection term (characteristic of an itinerant-electron system) must then be included in the appropriate surface perturbation $\hat{W}$ in (31).

Using (36), Mathon[2] argued that the spin-wave resolvent is given by

$$\Gamma_G(l_z,l_z') = \Gamma_B(|l_z - l_z'|) - \Gamma_B(|l_z + l_z'|) \ , \tag{37}$$

which has the same form as the spin-wave Green's function for a semi-infinite Heisenberg ferromagnet when one neglects changes in the exchange interactions near the surface. At least in the case of a strong ferromagnet, Mathon was then able to show that the secular equation (32) had the same form as in a Heisenberg ferromagnet, which is known to satisfy spin-rotational invariance (and hence exhibit the correct zero-frequency Goldstone mode) and which can be solved.[6] The disadvantage of this approach is that it is apparently limited to a specific limit with only *nn* interactions and where the classical reflection term is unimportant. For more general itinerant-electron ferromagnets, we believe our approach based on isolating the CIBM part of χ^0_{+-} may have advantages and that our new sum rule (15) will be useful in finding acceptable approximations to the surface perturbation $\hat{W}_S$ localized to the first few surface layers. However, such calculations are quite complicated and we defer further discussion to a future publication.

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