Ferromagnetism from Undressing

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We have recently proposed that superconductivity may be understood as driven by the undressing of quasiparticles as the superconducting state develops. Similarly we propose here that ferromagnetism in metals may be understood as driven by the undressing of quasiparticles as the ferromagnetic state develops. In ferromagnets, the undressing is proposed to occur due to the reduction in bond charge caused by spin polarization, in contrast to superconductors where the undressing is proposed to occur due to the reduction in site charge caused by (hole) pairing. The undressing process manifests itself in the one and two-particle Green’s functions as a transfer of spectral weight from high to low frequencies. Hence it should have universal observable consequences in one- and two-particle spectroscopies such as photoemission and optical absorption.

I. INTRODUCTION

The concept of a quasiparticle is central to our understanding of the physics of many-electron systems \[1,2\]. A quasiparticle is what remains of a particle (electron) after taking into account its interaction with surrounding particles. It may be understood as a particle carrying with it a ‘cloud’ of other particles with which it interacts. This cloud can be visualized as ‘clothing’, or ‘dressing’, of the original particle, and naturally it will generally lead to an increased effective mass of the quasiparticle.

In addition to the effective mass, another central element of the concept of a quasiparticle is its ‘weight’. Paradoxically, the ‘weight’ of a quasiparticle is usually the inverse of its effective mass. If a particle is heavily dressed by interactions, its effective mass is large and its ‘quasiparticle weight’ is small. The ‘quasiparticle weight’, \(Z\), expresses how much of the particle still remains intact, with a well-defined energy versus momentum relation. If \(Z\) is small, the particle has lost most of its identity; by a sum rule, this lost weight reappears elsewhere, in an incoherent background.

To recall the origin of the key connection between quasiparticle weight and its effective mass let us remember some basic concepts of many-body theory. Consider the Green’s function for a spin \(\sigma\) electron in a many-body system

\[
G(k, \tau) = \langle -Tc_{k\sigma}(\tau)c_{k\sigma}^\dagger(0) \rangle .
\]

\(G\) gives the probability amplitude to find an electron of momentum \(k\) at time \(\tau\) after it was created at time 0. Qualitatively, if the electron does not interact with anything it will be found in its entirety at time \(\tau\) with the same momentum \(k\) as when it was created at time 0. However if the electron interacts strongly with other degrees of freedom, we will find very little of it back at any later time. In that case the electron has lost its ‘coherence’, most or all of it has been lost in an incoherent background. This is why the Green’s function in a many-body system is generally written as

\[
G(k, \omega) = G_{\text{coh}}(k, \omega) + G'(k, \omega) \tag{2}
\]

where \(G_{\text{coh}}\), the coherent part of the Green’s function, represents the quasiparticle, and \(G'\) describes the incoherent background. This can be understood as follows. The exact Green’s function can be written as

\[
G(k, \omega) = \frac{1}{\omega - \epsilon_k - \Sigma(k, \omega)} \tag{3}
\]

where \(\Sigma\) is the self-energy, and \(\epsilon_k\) is its kinetic energy measured from the chemical potential, inversely proportional to its mass. Assume for simplicity that the self-energy has no \(k\)-dependence, and we have for its real part for small \(\omega\)

\[
\Sigma_{re}(\omega) = \Sigma_{re}(0) + \omega \frac{\partial \Sigma_{re}}{\partial \omega} \tag{4}
\]
The imaginary part of the self-energy and gives rise to the incoherent contribution. Thus, Eq. (5) shows that the same factor \( Z \), the wave function renormalization factor, determines the quasiparticle spectral weight and the effective mass renormalization.

This deep connection between quasiparticle weight and its effective mass is well known. However it has not been stressed in the recent literature. For example, there is a vast recent literature on the phenomenon of colossal magnetoresistance in manganites, where the transition to the ferromagnetic state is thought to be accompanied by a reduction in the carrier’s effective mass. Yet there has been no discussion to our knowledge of any corresponding change in the quasiparticle weight. Here we will make such a connection, for the manganites and for ferromagnetic metals in general.

We have pointed out in the past that within a class of model Hamiltonians both superconductivity and ferromagnetism may be understood as driven by a lowering of the carrier’s effective mass as the ordered state develops, or equivalently a lowering of the carrier’s kinetic energy, and proposed that this common aspect of the physics may be essential to both phenomena. Only recently however have we focused on the fundamental connection between the lowering of effective mass and the corresponding expected increase in the quasiparticle weight, or ‘undressing’, for the case of superconductivity (hereafter referred to as I). This connection was brought to the limelight by the beautiful experimental results and insightful analysis of Ding et al. on photoemission in cuprates, as well as experimental work by Feng et al. and Basov et al. Here we make this connection for the case of ferromagnetism. It leads to a remarkably simple picture of metallic ferromagnetism, and to the understanding that both ferromagnetism and superconductivity may be driven by the same physical principle: undressing.

II. THE PHYSICS

Consider the process of creating an electron of spin \( \uparrow \) at site \( i \). Imagine there is an electron of spin down at the bond connecting site \( i \) to a neighboring site \( j \), as shown in Fig. 1. The \( \downarrow \) electron is in state \( |0\rangle \), its ground state, in the absence of occupation of site \( i \). The strong Coulomb repulsion between like charges will affect the state of that bond charge. When the \( \uparrow \) electron is created at site \( i \), the \( \downarrow \) electron will make a transition to one of the bond states \( |1\rangle \), the eigenstates of the bond \( \downarrow \) electron in the presence of an \( \uparrow \) electron at site \( i \). Let the ground state of that manifold be \( |1\rangle = \sum_{i} |1\rangle^{\uparrow} |0\rangle \), and we denote by

\[
S = <0|1>
\]

the overlap matrix element of the ground states of the \( \downarrow \) bond electron in the absence and in the presence of an \( \uparrow \) electron at site \( i \). We can express this mathematically as

\[
|1\rangle^{\uparrow} |0\rangle = |\uparrow\rangle |0\rangle = \sum_{l} |\uparrow\rangle |1l\rangle = \sum_{l \neq 0} |\uparrow\rangle |1l\rangle = \sum_{l \neq 0} |\uparrow\rangle |1l\rangle^{\uparrow} |0\rangle
\]

Here, the first ket denotes the electronic state of the site \( i \), and the second ket denotes the state of the \( \downarrow \) electron at the bond. The first term in Eq. (8), where the \( \downarrow \) electron ends up in its ground state \( |1\rangle \), represents a coherent process that preserves the phase of the wave function. It is a ‘diagonal transition’ in the language of small polaron theory. If instead the \( \downarrow \) electron at the bond ends up in an excited state, it represents an incoherent process (non-diagonal transition). The overlap matrix element \( S \) represents what fraction of the \( \uparrow \) electron created at site \( i \) remains coherent, and gives rise to its reduced quasiparticle ‘weight’. If \( S \) is very small it means most of the effect of the \( \uparrow \) electron creation has been dissipated in incoherent processes that left the ‘background’ \( \downarrow \) electron in excited states.

If instead we create the \( \uparrow \) electron at site \( i \) when there is no electron at bond \( ij \) we have simply

\[
\Sigma_{\gamma}(0) \text{ just renormalizes the chemical potential. From general phase space arguments one knows that the imaginary part of } \Sigma \text{ goes to zero as } \omega^{2} \text{ for small } \omega. \text{ Hence we can separate the low frequency real part of the Green’s function and obtain}
\]

\[
G(k, \omega) = \frac{1}{\omega(1 - \frac{\partial \Sigma_{\omega}}{\partial \omega}) - \epsilon_{k}} + G' = \frac{Z}{\omega - Z \epsilon_{k}} + G'
\]

with

\[
Z = \frac{1}{1 - \frac{\partial \Sigma_{\omega}}{\partial \omega}}
\]
\[ c^\dagger_{i\uparrow}|0> = |\uparrow> \] (9)

and no incoherent piece is generated, because there was no 'background' degree of freedom to excite; hence, the weight of the quasiparticle is 1 in this case.

More generally, we could instead have an \( \uparrow \) electron on the bond, or both \( \uparrow \) and \( \downarrow \) electrons. We argue that Eq. (8) still applies, with the second ket denoting the state of the total charge at the bond. If there is no charge at the bond, Eq. (9) instead applies. We define then a quasiparticle operator \( \tilde{c}_{i\uparrow} \) through the relation

\[ c^\dagger_{i\uparrow} = [1 - (1 - S)\tilde{n}_{ij\sigma} + \tilde{n}_{ij\sigma}]\tilde{c}^\dagger_{i\uparrow} \] (10)

where \( \tilde{n}_{ij\sigma} \) is the bond occupation number (0 or 1) of the spin \( \sigma \) electron. Eq. (10) is only the coherent part of the electron operator, as it does not generate the second ket of Eq. (8) (we use the same operator notation on the left for simplicity only). Eq. (10) restates Eqs. (8) and (9), that the weight of \( c^\dagger_{i\uparrow} \) is 1 if the neighboring bond is unoccupied, and it is maximally reduced to \( S < 1 \) if the neighboring bond is occupied by spin \( \uparrow \) and \( \downarrow \) electrons.

The physics resulting from these equations is shown schematically in Fig. 2. As in I, we use an 'independent boson model' with an Einstein oscillator [11] to describe the coupling of the electron at site \( i \) to the excited states of the charge (in this case the bond charge) shown in Fig. 1. The coherent part of the spectral function (quasiparticle peak, labeled q.p.) arises from the ground-state to ground-state transition of the oscillator when the electron is created at the site, and its height is the quasiparticle weight \( Z \). \( Z \) increases as the bond charge decreases, and correspondingly weight in the spectral function shifts from the incoherent part to the quasiparticle peak. As we will show in the next section, the bond charge decreases when spin polarization develops.

If instead of focusing on the bond charge we were to focus on the site charge the equation analogous to (10) is

\[ c^\dagger_{i\sigma} = [1 - (1 - S)\tilde{n}_{ij\sigma} + \tilde{n}_{ij\sigma}]\tilde{c}^\dagger_{i\sigma} \] (11)

where \( \tilde{n}_{ij\sigma} \) is the site charge occupation. It was shown in I that Eq. (11) leads to superconductivity through undressing.

Next we wish to express the bond charge in terms of electron operators. We use the operator representation

\[ \tilde{n}_{ij\sigma} = \tilde{c}^\dagger_{i\sigma} \tilde{c}_{j\sigma} + \tilde{c}^\dagger_{j\sigma} \tilde{c}_{i\sigma} \] (12)

which has eigenvalue 1 operating on the low energy bonding state

\[ |\sigma > |0 > + |0 > |\sigma > \] (13)

and zero if the bonding state is empty. Eq. (10) is then

\[ c^\dagger_{i\uparrow} = [1 - (1 - S)\frac{1}{2} \sum_{\sigma} (\tilde{c}^\dagger_{i\sigma} \tilde{c}_{j\sigma} + \tilde{c}^\dagger_{j\sigma} \tilde{c}_{i\sigma})] \tilde{c}^\dagger_{i\uparrow} \] (14)

Eq. (14) is the analog, for the effect of creating the \( \uparrow \) electron on site \( i \) on the neighboring bond charge, to Eq. (11) for the effect of creating the \( \uparrow \) electron on site \( i \) on the site charge. Note an important difference: under a particle-hole transformation

\[ c^\dagger_{i\sigma} \rightarrow (-1)^i c^\dagger_{i\sigma} \] (15)

(on a bipartite lattice) Eq. (14) is invariant, while Eq. (11) changes to

\[ c^\dagger_{i\sigma} = [S + (1 - S)\tilde{n}_{ij\sigma} \tilde{c}^\dagger_{i\sigma}] \] (16)

Eq. (11) implies that increasing electron site concentration leads to increased dressing of electrons, and conversely Eq. (16) implies that increasing hole site concentration leads to undressing of holes. Instead, Eq. (14) and its identical form in hole representation imply that increasing bond occupation leads to increased dressing, both for electrons and holes. This difference between the dressing effects of site and bond charges lies at the root of the difference between superconductivity and ferromagnetism.

Finally, we consider a d-dimensional hypercubic lattice and add the contributions from all the bonds connecting to a given site, and Eq. (14) becomes

\[ c^\dagger_{i\sigma} = [1 - (1 - S)\frac{1}{2} \sum_{\delta,\sigma'} (\tilde{c}^\dagger_{i\sigma} \tilde{c}_{i+\delta\sigma'} + \tilde{c}^\dagger_{i+\delta\sigma'} \tilde{c}_{i\sigma'})] \tilde{c}^\dagger_{i\sigma} \] (17)

We explore its consequences in the next sections.
III. QUASIPARTICLE HAMILTONIAN

Consider the kinetic energy operator on a lattice

\[ H_{\text{kin}} = - \sum_{i,j,\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} \]  

(18)

Replacing the bare electron operators in Eq. (18) by the quasiparticle operators Eq. (17) yields the low energy effective Hamiltonian for quasiparticles

\[ H_{\text{kin}} = - \sum_{i,j,\sigma} t_{ij} \times \]

\[ \left[ 1 - \frac{(1 - S)}{2} \sum_{\delta,\sigma',t} (c_{i\sigma}^\dagger \tilde{c}_{i+\delta\sigma'} + c_{i+\delta\sigma'}^\dagger \tilde{c}_{i\sigma}) \right] c_{i\sigma}^\dagger \tilde{c}_{j\sigma} \left[ 1 - \frac{(1 - S)}{2} \sum_{\delta,\sigma',t} (c_{j\sigma}^\dagger \tilde{c}_{j+\delta\sigma'} + c_{j+\delta\sigma'}^\dagger \tilde{c}_{j\sigma}) \right] \]  

(19)

In expanding this expression we will ignore terms involving more than two centers for simplicity, as well as terms with more than four fermion operators. The latter can certainly be rigorously justified if the electron (or hole) density is low. Eq. (19) then becomes

\[ H_{\text{kin}} = - \sum_{i,j,\sigma} t_{ij} c_{i\sigma}^\dagger \tilde{c}_{j\sigma} + (1 - S) \sum_{\langle i,j \rangle} t_{ij} \left( \sum_{\sigma} c_{i\sigma}^\dagger \tilde{c}_{j\sigma} + \text{h.c.} \right)^2 \]  

(20a)

which can also be written as

\[ H_{\text{kin}} = - \sum_{i,j,\sigma} t_{ij} c_{i\sigma}^\dagger \tilde{c}_{j\sigma} + 2(1 - S) \sum_{i,j,\sigma'} t_{ij} c_{i\sigma}^\dagger c_{j\sigma}^\dagger \tilde{c}_{j\sigma'}^\dagger \tilde{c}_{i\sigma'} + 2(1 - S) \sum_{i,j,\sigma',t} t_{ij} c_{i\sigma}^\dagger c_{j\sigma}^\dagger \tilde{c}_{j\sigma'}^\dagger \tilde{c}_{j\sigma} \]  

(20b)

In the form Eq. (20a), the interaction term generated can be simply understood as bond-charge Coulomb repulsion [13]. In the form Eq. (20b) it can be seen that the two interaction terms are precisely of the same form as the exchange and pair hopping terms that result from considering off-diagonal matrix elements of the Coulomb interaction in a tight binding representation [13].

\[ J_{ij} = \int d^3 r d^3 r' \phi_i^*(r) \phi_j^*(r') \frac{e^2}{|r - r'|} \phi_i(r) \phi_j(r) \]  

(21a)

\[ J'_{ij} = \int d^3 r d^3 r' \phi_i^*(r) \phi_j^*(r') \frac{e^2}{|r - r'|} \phi_j(r) \phi_j(r) \]  

(21b)

In general, we will have \( J = J' \) from Eq. (21) if the wavefunctions can be assumed to be real. Eq. (20) implies

\[ J_{ij} = J'_{ij} = 2t_{ij} (1 - S) \]  

(22)

Supplementing the kinetic energy with an on-site Coulomb repulsion leads to the low energy effective Hamiltonian

\[ H = - \sum_{\langle i,j \rangle,\sigma} t_{ij} (\tilde{c}_{i\sigma}^\dagger \tilde{c}_{j\sigma} + \text{h.c.}) \left( \hat{n}_{i\uparrow} + \hat{n}_{i\downarrow} \right) \]

\[ + \sum_{i,j,\sigma',t} J_{ij} c_{i\sigma}^\dagger \tilde{c}_{j\sigma'}^\dagger \tilde{c}_{j\sigma'}^\dagger \tilde{c}_{i\sigma} + \sum_{i,j,\sigma',t} J'_{ij} c_{i\sigma}^\dagger \tilde{c}_{i\sigma'}^\dagger \tilde{c}_{j\sigma}^\dagger \tilde{c}_{j\sigma'} \]  

(23)

to describe the dynamics of the quasiparticles.

We have extensively studied the properties of this Hamiltonian for nearest neighbor hopping \( t_{ij} = t \) and interactions \( J_{ij} = J, J'_{ij} = J' \), in particular for the cases \( J' = 0 \) and \( J' = J \). The ‘exchange term’ involving \( J \) can also be written as

\[ H_j = -2J \sum_{\langle i,j \rangle} (\vec{S}_i \cdot \vec{S}_j + \frac{1}{4} \hat{n}_i \hat{n}_j) \]  

(24a)

with
and $\sigma_\alpha$ a Pauli matrix ($\alpha = x, y, z$). In the form Eq. (24) it looks like a 'Heisenberg exchange' term. However, as emphasized earlier [4,14], the origin of ferromagnetism here is not quantum-mechanical exchange of localized spins, as in Heisenberg’s case. The combination of the $J$ and $J'$ terms in the form Eq. (20a) displays the origin of these interactions as bond-charge Coulomb repulsion. Ferromagnetism in this model is driven by reduction of bond-charge Coulomb repulsion as spin polarization develops and accompanying kinetic energy lowering, rather than quantum-mechanical exchange.

The properties of the model Eq. (23) for nearest neighbor hoppings and interactions

$$H = -t \sum_{\langle ij \rangle, \sigma} (\hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} + \text{h.c.}) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} + J \sum_{i, j, \sigma \sigma'} \hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} \hat{c}^\dagger_{j\sigma} \hat{c}_{i\sigma} + J' \sum_{i, j, \sigma \sigma'} \hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} \hat{c}^\dagger_{j\sigma} \hat{c}_{i\sigma}$$

are similar for different values of $J'/J$ [4,14,19]. In particular, within mean field theory and for a model with constant density of states, the conditions on the parameters for ferromagnetism to occur are

$$j > \frac{1 - u}{2 - m^2 - (1 - n)^2}$$

(26a)

$$j > \frac{1 - u}{\frac{5}{3} - \frac{3}{2}m^2 - \frac{1}{2}(1 - n)^2}$$

(26b)

for $J' = 0$ and for $J' = J$ respectively, with

$$u = U/D$$

(27a)

$$j = zJ/D$$

(27b)

$$j' = zJ'/D$$

(27c)

Here, $m$ is the magnetization per site, $n$ the total occupation per site, $z$ the number of nearest neighbors to a site and $D = 2zt$ the bare bandwidth. In particular, for the half-filled band ($n = 1$) the condition for full spin polarization ($m = n$) is

$$j = \frac{J}{2t} > 1 - u$$

(28)

in both cases. For $U = 0$, this condition is achieved in the limit $S \to 0$ according to Eq. (22), while for increasingly larger $U$ smaller values of $J$ are required, and hence larger values of $S$ are sufficient. Exact diagonalization studies of the Hamiltonian Eq. (25) show that the mean field conditions Eq. (26) are qualitatively correct and reasonably accurate particularly for the half-filled band and not too large values of $U$ [14].

In what follows we will for simplicity consider the model with $J$ only:

$$H = -t \sum_{\langle ij \rangle, \sigma} (\hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} + \text{h.c.}) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} + J \sum_{i, j, \sigma \sigma'} \hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} \hat{c}^\dagger_{j\sigma} \hat{c}_{i\sigma} + J' \sum_{i, j, \sigma \sigma'} \hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} \hat{c}^\dagger_{j\sigma} \hat{c}_{i\sigma}$$

(29)

One argument for dropping the $J'$ term is that its importance is suppressed due to on-site Coulomb repulsion. However, in treating the Hamiltonian in mean field theory this effect may not be properly taken into account. The effective kinetic energy that results from Eq. (29) within mean field theory is

$$\epsilon_{k\sigma} = (1 - 2j(I_\uparrow + I_\downarrow))\epsilon_k$$

(30a)

with

$$I_\sigma = <\hat{c}^\dagger_{i\sigma} \hat{c}_{i+s,\sigma}>$$

(30b)

(one half of) the average bond charge for spin $\sigma$. $\epsilon_k$ is the Fourier transform of the bare hopping amplitude $t_{ij}$. For a model with a constant density of states, the average bond charge at zero temperature is given by.
so that it decreases with increasing magnetization, as expected.

The properties of the model are simplest in the half-filled band case, and we will restrict ourselves to that case in what follows. For that case,

$$I_\uparrow = I_\downarrow = \frac{I}{2}$$

(32)
even in the presence of spin polarization. As the temperature is lowered below $T_c$ and ferromagnetism develops, the average bond charge decreases for both majority and minority spins [4], and the effective bandwidth

$$D_{eff} = (1 - 2jI)D$$

(33)
broadens. In the normal state, as the temperature decreases the bond charge occupation Eq. (30b) increases and hence the bandwidth narrows. The temperature and magnetization dependence of the bond charge leads to a variety of interesting properties of the mean field solution of this model that are not found in the Stoner model, i.e. the mean field solution of the repulsive Hubbard model, and that describe experimental observations, as discussed in the references [4].

What is the significance of having derived the Hamiltonians Eq. (23) or Eq. (25) in this new way? Twofold. First, if one assumes that the interactions $J$ and $J'$ in Eq. (23) arise from off-diagonal matrix elements of the Coulomb interaction as given by Eq. (21), their value is expected to be rather small. This is because one has to use properly orthogonalized atomic orbitals in Eq. (21). When the Mulliken approximation [17] holds, which is usually the case, off-diagonal matrix elements such as $J$ and $J'$ are very small for orthogonalized orbitals, and this is the justification for the ‘zero differential overlap’ approximation in quantum chemistry [18]. However, there is a more fundamental reason why the present derivation of the Hamiltonian Eq. (23) is more satisfactory than the one using the Coulomb matrix elements argument. This is discussed in the next section.

IV. FERROMAGNETISM AND SPECTRAL WEIGHT TRANSFER

The single particle Green’s function (for spin $\uparrow$ electrons) is given by

$$G_{ij}(\tau) = \langle -T c_{i\uparrow}(\tau)c_{j\uparrow}^\dagger(0) \rangle = G_{ij}^{coh}(\tau) + G_{ij}^{incoh}(\tau)$$

(34)
with $T$ the time ordering operator. The coherent and incoherent parts of the Green’s function arise from the first and other terms in Eq. (8) respectively. For the coherent part, we replace the electron operators in terms of quasiparticle operators and obtain

$$G_{ij}^{coh}(\tau) = \langle -T[1 - (1 - S)\tilde{n}_{bond,i}(\tau)]\tilde{c}_{i\uparrow}(\tau)\tilde{c}_{i\downarrow}^\dagger(0)[1 - (1 - S)\tilde{n}_{bond,j}(0)] \rangle$$

(35)
where $\tilde{n}_{bond,i}$ represents the bond charge adjacent to site $i$. A mean field decoupling leads to

$$G^{coh}_{ij}(\tau) = [1 - (1 - S)\langle \tilde{n}_{bond} \rangle] \langle -T\tilde{c}_{i\uparrow}(\tau)\tilde{c}_{i\downarrow}^\dagger(0) \rangle = Z \langle -T\tilde{c}_{i\uparrow}(\tau)\tilde{c}_{i\downarrow}^\dagger(0) \rangle$$

(36)
Equation (36) defines the quasiparticle weight $Z$. We take for the average bond charge

$$\langle \tilde{n}_{bond} \rangle = \sum_\sigma \langle c_{i\sigma}^\dagger c_{j\sigma} + h.c. \rangle = 2(I_\uparrow + I_\downarrow)$$

(37a)
which can be written as [4]

$$I = \int_{-D/2}^{D/2} d\epsilon g(\epsilon)(-\frac{\epsilon}{D/2})[f(\epsilon_\uparrow(\epsilon) + f(\epsilon_\downarrow(\epsilon))] \equiv I(T, m)$$

(37b)
and is a function of temperature and magnetization. Here, $\epsilon_\sigma(\epsilon)$ are the quasiparticle energies and $g(\epsilon)$ the density of states. Hence the quasiparticle weight is simply

$$Z = Z(T, m) = 1 - 2(1 - S)I(T, m) = 1 - 2jI(T, m)$$

(38)
and will depend on temperature and magnetization through the temperature and magnetization dependence of the bond charge. Note that for a more general case with a non-half-filled band, one would have different quasiparticle weights $Z_\sigma$ for spin up and down electrons in the spin-polarized state. Such a situation is also easily treated within this framework.

We consider the mean field solution of the model Eq. (29). The quasiparticle energies are given by

$$\epsilon_{k\sigma} = \epsilon_\sigma(\epsilon_k) = (1 - 2 J I) \epsilon_k - \frac{U + J z}{2} m - \mu$$  \hspace{1cm} (39)

where the magnetization $m$ and chemical potential $\mu$ are determined by the conditions

$$m = \int_{-D/2}^{D/2} d\epsilon g(\epsilon)[f(\epsilon \uparrow(\epsilon)) - f(\epsilon \downarrow(\epsilon))]$$  \hspace{1cm} (40a)

$$n = \int_{-D/2}^{D/2} d\epsilon g(\epsilon)[f(\epsilon \uparrow(\epsilon)) + f(\epsilon \downarrow(\epsilon))]$$  \hspace{1cm} (40b)

with $n$ the carrier concentration. From Eq. (39), the effective bandwidth is given by

$$D_{eff} = (1 - 2 J I) D = [1 - 2(1 - S) I] D$$  \hspace{1cm} (41)

where for the last equality we have used Eqs. (22) and (27b). The effective mass is given by

$$\frac{m^*}{m_0} = \frac{1}{1 - 2 J I}$$  \hspace{1cm} (42)

where $m_0$ is the bare mass determined by the bare hopping amplitude in Eq. (18). From Eqs. (38) and (42) we have simply

$$\frac{m^*}{m} = \frac{1}{Z(T, m)}$$  \hspace{1cm} (43)

as expected from Eq. (5).

The behavior of $I(T, m)$ is discussed in the references [4]. In Fig. 3 we reproduce a representative case. As the temperature is lowered in the normal state $I(T, m)$ increases, and it decreases again as spin polarization develops. Correspondingly, the bandwidth $D_{eff}$ decreases in the normal state upon cooling and expands again as the ordered state develops; similarly the quasiparticle weight $Z$ decreases above $T_c$ as $T$ decreases, and increases as spin polarization develops. If no magnetization were to develop, for the parameters in Fig. 3 the effective bandwidth would shrink to zero as the temperature goes to zero.

The coherent part of the spectral function is given by

$$A_{\sigma coh}(k, \omega) = -\frac{1}{\pi} \text{Im} G_{coh}(k, \omega + i\delta) = Z \delta(\omega - \epsilon_{k\sigma})$$  \hspace{1cm} (44)

We can model the full spectral function by assuming a harmonic oscillator spectrum of frequency $\omega_0$ associated with the bond charge excitations at each bond in Eq. (8). The result is

$$A_\sigma(k, \omega) = Z \delta(\omega - \epsilon_{k\sigma})$$

$$+ Z \sum_{l=1}^{\infty} \frac{(ln Z)^l}{l!} \frac{1}{N} \sum_{k'} [n_{k'} \delta(\omega + l\omega_0 - \epsilon_{k'\sigma}) + (1 - n_{k'}) \delta(\omega - l\omega_0 - \epsilon_{k'\sigma})]$$  \hspace{1cm} (45)

which is easily seen to satisfy the sum rule

$$\int_{-\infty}^{\infty} d\omega A_\sigma(k, \omega) = 1$$  \hspace{1cm} (46)

and describes the transfer of spectral weight from high to low frequencies as the quasiparticle weight $Z$ (Eq. (38) increases when spin polarization develops. Similarly, the optical sum rule states
\[ \int_0^{\omega_m} d\omega \sigma_1(\omega) = \frac{\pi e^2 n}{2m^*} \]  

(47)

for the intra-band spectral weight of the optical conductivity \( \sigma_1(\omega) \). In Eq. (47), \( \omega_m \) is a high frequency cutoff that excludes transitions to other bands. Using Eq. (43),

\[ \int_0^{\omega_m} d\omega \sigma_1(\omega) = \frac{\pi e^2 n}{2m_0} Z(T, m) \]  

(48)

so that as the system becomes more coherent with increasing \( Z \), spectral weight is also transferred into the intra-band part of the optical conductivity. If Eq. (47) is integrated to infinity however

\[ \int_0^{\infty} d\omega \sigma_1(\omega) = \frac{\pi e^2 n}{2m_0} Z(T, m) (49) \]

with \( m_0 \) the bare mass. Thus, the extra spectral weight that goes into intraband optical absorption has to be compensated by a corresponding decrease in the incoherent contribution so as to leave Eq. (49) invariant.

In the presence of a magnetic field the quasiparticle energies are

\[ \epsilon_\sigma(\epsilon) = (1 - 2jI)\epsilon - \sigma(\frac{U + J_z}{2} m + Dh) - \mu \]  

(50)

with \( h \) a dimensionless magnetic field. Increasing \( h \) gives rise to increasing magnetization and decreasing bond charge \( I \), as seen in Fig. 3. Hence, the quasiparticle weight increases and the effective mass decreases. The magnetoresistance in this model is given by

\[ \frac{\Delta \rho}{\rho} = \frac{\rho(h) - \rho(0)}{\rho(0)} = 2jI(T, m(h)) - I(T, m(0)) \]  

(51)

and its behavior with temperature and magnetic field resembles that seen in ferromagnets [4]. From the Drude form for the intra-band optical conductivity

\[ \sigma_1(\omega) = \frac{ne^2}{m^*} \frac{\tau}{1 + \omega^2 \tau^2} = \frac{ne^2}{m_0} Z(T, m) \frac{\tau}{1 + \omega^2 \tau^2} \]  

(52)

we conclude that the intra-band conductivity will increase with application of a magnetic field, and correspondingly the high frequency conductivity from incoherent processes will decrease. To model both parts of the conductivity we take as a simple Ansatz the spectral density Eq. (45) ignoring the momentum dependence

\[ \sigma_1(\omega) = \frac{ne^2}{m_0} Z(T, m)[\frac{\tau}{1 + \omega^2 \tau^2} + \frac{\pi}{2} \sum_{l=1}^{\infty} \frac{(ln \frac{1}{l})^l}{l!} \delta(\omega - l\omega_0)] \]  

(53)

which properly satisfies the sum rules Eqs. (48) and (49). In figure 4 we show examples of the behavior expected under variation of magnetic field and temperature. Qualitatively similar behavior is seen in the optical properties of colossal magnetoresitive manganites [21] and of europium hexaboride [22].

Similarly, we expect the enhanced coherence in the ferromagnetic state to be displayed in angle-resolved photoemission experiments: under application of a magnetic field or lowering the temperature in the ferromagnetic state, quasiparticle peaks should become stronger reflecting the enhanced quasiparticle weight \( Z(T, m) \). We will present quantitative analysis and comparison with experiment elsewhere.

V. PUZZLES WITH THE OPTICAL SUM RULE

The optical sum rule in tight binding models needs to be treated with some care. Consider the quasiparticle Hamiltonian Eq. (29). According to the discussion in the previous section, within mean field theory Eq. (42) gives rise to a lowering of effective mass as spin polarization develops, hence to an increased intra-band optical spectral weight according to Eq. (47).

However, the polarization operator on the lattice is given by [23]
\[ \vec{P} = e \sum_i \vec{R}_i n_i \]  

(54)

with \( R_i \) the position vector for site \( i \). The current operator (in direction \( \delta \)) is obtained from its time derivative

\[ J_\delta = \frac{dP_\delta}{dt} = \frac{i}{\hbar} [H, P_\delta] \]  

(55)

and is easily seen to be independent of \( J \), because the exchange term in Eq. (29) carries no current. Hence the exact intra-band optical sum rule for this Hamiltonian is [24]

\[ \int_0^{\omega_m} d\omega \sigma_1(\omega) = \frac{\pi a^2 e^2}{2\hbar^2} < -T_\delta^I > \]  

(56a)

\[ < -T_\delta^I > = t \sum < \hat{c}_{i}^{\dagger} \hat{c}_{i+\delta} + \text{h.c.} > \]  

(56b)

Eq. (56) predicts that as spin polarization develops and the bond charge decreases the intra-band spectral weight will decrease. This qualitatively contradicts the prediction of mean field theory for this very same model, as well as the expectation based on the physical considerations of the previous section. We are thus led to the remarkable conclusion that the exact solution of the model Eq. (29) does worse than its mean field solution in capturing essential aspects of its physics.

The situation can be remedied to some extent by including the pair hopping term in the Hamiltonian. That term does carry a current, and the sum rule Eq. (56) becomes [25]

\[ \int_0^{\omega_m} d\omega \sigma_1(\omega) = \frac{\pi a^2 e^2}{2\hbar^2} [< -T_\delta^I > + 4 < -T_\delta^{J'-I} >] \]  

(57a)

\[ < -T_\delta^{J'-I} > = -J' \sum_{i,\sigma} < \hat{c}_{i+\delta,\sigma}^{\dagger} \hat{c}_{i,\sigma}^{\dagger} \hat{c}_{i,\sigma} \hat{c}_{i+\delta,\sigma} > \]  

(57b)

In the normal state the expectation value Eq. (57b) is negative and as spin polarization develops it will decrease in magnitude leading to an increase in the optical spectral weight, in accordance with qualitative expectation. These considerations illustrate that the optical sum rule places severe constraints on what acceptable effective low energy Hamiltonians are and on the relative magnitude of their parameters. The subject clearly needs further investigation which is outside the scope of this paper.

VI. CONCLUSIONS

This paper started from the assumption that the electron creation operator at site \( i \) can be represented as

\[ c_{i\uparrow}^\dagger = [1 - (1 - S)\hat{n}(\text{bond})] c_{i\uparrow}^\dagger + \text{incoherent part} \]  

(58a)

where the ‘incoherent part’ contains excitations of the local bond charge, and \( S \) describes the overlap of the bond-charge configuration ground state in the presence and absence of the \( \uparrow \) electron at site \( i \). Similarly, the work of I was based on the assumption that the operator can be represented as

\[ c_{i\uparrow}^\dagger = [1 - (1 - S)\hat{n}(\text{site})] c_{i\uparrow}^\dagger + \text{incoherent part} \]  

(58b)

More generally then we conclude that a general representation should be

\[ c_{i\uparrow}^\dagger = [1 - (1 - S)\hat{n}(\text{local})] c_{i\uparrow}^\dagger + \text{incoherent part} \]  

(58c)

where \( \hat{n}(\text{local}) \) includes nearby site and bond charges. We have shown in I that Eq. (58a) leads to superconductivity, and here that Eq. (58b) leads to ferromagnetism. More generally, Eq. (58c) will lead to a unified description of superconductivity and ferromagnetism where one or the other (or neither) will dominate depending on characteristics of the system such as nature of the orbitals, lattice structure and band filling.
In connection with superconductivity we note that in I the nature of the boson degree of freedom was left somewhat unspecified. The analogy with the situation discussed here makes it unambiguous that the boson degree of freedom there is also electronic, as described e.g. by the electronic model with two orbitals per site \cite{26}, rather than e.g. a high frequency phonon.

The physics of ferromagnetism that results from Eq. (58a), and that of superconductivity that results from Eq. (58b), are remarkably alike: onset of the ordered state leads to increased quasiparticle coherence. Spectral weight, both in the one-particle properties such as photoemission, and in two-particle properties such as optical absorption, is transferred from the incoherent high frequency background to the low frequency coherent response. Quasiparticles undress, and become more like free particles, as the ordered state develops.

Remarkably, the quasiparticle Hamiltonians that result from Eqs. (58a) and (58b) lead respectively to the various off-diagonal matrix elements of the Coulomb interaction in a local representation \cite{12}: Eq. (58a) to exchange and pair hopping (or equivalently bond-bond-charge repulsion), and Eq. (58b) to correlated hopping (or bond-site charge repulsion). In our earlier work we had shown that these off-diagonal matrix elements lead to metallic ferromagnetism \cite{4} and hole superconductivity \cite{3} respectively, and that the common aspect of the physics of both instabilities induced by these interactions is effective mass reduction, which through the optical sum rule implies transfer of optical spectral weight to low frequencies. However, thinking about those interaction terms as simply derived from static matrix elements of the Coulomb interaction does not lead to an understanding of the optical spectral weight transfer process, nor to the understanding that spectral weight transfer should also occur in the one-particle Green’s function. Instead, the point of view presented in this paper and in I does.

What is the evidence that the physics discussed here takes place in ferromagnetic metals? We have already mentioned that at least in some ferromagnetic metals \cite{21,22} there is evidence for optical spectral weight transfer from high to low frequencies as the ferromagnetic state develops, either by decreasing the temperature or by increasing the magnetic field \cite{27}. We are not aware that evidence for undressing physics has been seen yet in the single particle spectral function of ferromagnets, as would be detected in photoemission experiments, but expect that it should be observable at least in manganites and hexaborides. For ferromagnets that are more ‘metallic’ in the normal state, i.e. have higher coherence, it will be more difficult to detect these effects since the changes should be comparatively smaller.

As suggested earlier \cite{4} we believe the universal properties of negative magnetoresistance of ferromagnets and anomalously large decrease of resistivity below $T_c$ are evidence for effective mass reduction due to ‘undressing’, as described by this paper, rather than for reduction of spin disorder scattering as usually assumed \cite{28}. The difference is not semantics: in the Drude form for the optical conductivity, Eq. (52), changes in $\tau$ and in $m^*$ will lead to different behavior at non-zero frequencies, and it should be possible to decide this question experimentally.

We also mention that another argument in favor of the picture of ferromagnetism discussed here and in our earlier work is the anomalous thermal expansion seen in ferromagnets below $T_c$. This is clearly due to reduction of the bond charge as the systems become ferromagnetic \cite{29}, and points to the importance of the bond charge in the phenomenon of ferromagnetism as described by our theory.

We believe that an experimental effort to detect the existence of undressing in itinerant electron systems that become ferromagnetic should be undertaken. There will of course be many system where such evidence may be too small to be experimentally detectable. However, if the evidence is found in a variety of different itinerant ferromagnets it will provide convincing evidence that the universal principle governing the transition to ferromagnetism in metals is undressing. The fact that it may be possible to also understand superconductivity with the same physical principle \cite{6} lends further support to the possibility that ‘undressing’ may capture the essential physics of both phenomena.

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\end{enumerate}
FIG. 1. When the spin $\uparrow$ electron is created at site $i$, the state of the bond charge between sites $i$ and $j$, represented here by a $\downarrow$-spin electron, changes because of Coulomb repulsion. It may make a diagonal transition to its new ground state $|1>$ (coherent process) or be left in an excited state $|1_l>$ (incoherent process).

FIG. 2. Schematic picture of the single particle spectral function resulting from the physics proposed here. In the unpolarized state (upper part) there is a large electronic bond charge density, most of the spectrum is incoherent and the quasiparticle weight $Z$, the height of the peak labeled q.p., is small. As spin polarization develops (lower part) the bond charge density is reduced, the quasiparticle weight increases and spectral weight in the incoherent part of the spectrum becomes smaller. For the example in the figure, $Z = 0.1$ for the upper part and $Z = 0.5$ for the lower part. Such qualitative features (albeit less extreme) should be seen in photoemission spectra of ferromagnetic metals.

FIG. 3. Characteristic behavior of the bond charge $I(T, m)$. Parameters used here are $j = 1$, $u = 0$, for $n = 1$. As the temperature is lowered above $T_c$ the bond charge increases, and when spin polarization develops below $T_c$ it decreases again. If no spin polarization is allowed to develop (dashed curve labeled $m = 0$) the bond charge continues increasing as $T$ is lowered, and correspondingly the effective bandwidth decreases, at a cost in kinetic energy. That cost is relieved by the development of spin polarization. In the presence of a magnetic field (Eq. (50)) (dash-dotted line) the magnetization increases and the bond charge is reduced.

FIG. 4. Characteristic behavior expected for the real part of the optical conductivity $\sigma_1(\omega)$ (arbitrary units), for the same parameters as in Fig. 3, with $D = 1eV$. The expression Eq. (53) is used, with $\omega_0 = 0.2eV$ and $\tau = 50eV^{-1}$. The $\delta$-functions in Eq. (53) were broadened to Lorentzians with half-width $\Gamma = 0.1eV$. Full line shows optical absorption at $T_c$ in the absence of a magnetic field. Both when the temperature is lowered (dashed line) and when a magnetic field is applied (dash-dotted line) spectral weight is transferred from the incoherent region to the low frequency Drude region due to the undressing induced by spin polarization.
Figure 1
Figure 2
Figure 3
