

QUASIPARTICLE UNDRRESSING: A NEW ROUTE TO COLLECTIVE EFFECTS IN SOLIDS

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Abstract. The carriers of electric current in a metal are quasiparticles dressed by electron-electron interactions, which have a larger effective mass m^* and a smaller quasiparticle weight z than non-interacting carriers. If the momentum dependence of the self-energy can be neglected, the effective mass enhancement and quasiparticle weight of quasiparticles at the Fermi energy are simply related by $z = m/m^*$ (m =bare mass). We propose that both superconductivity and ferromagnetism in metals are driven by quasiparticle 'undressing', i.e., that the correlations between quasiparticles that give rise to the collective state are associated with an increase in z and a corresponding decrease in m^* of the carriers. Undressing gives rise to lowering of kinetic energy, which provides the condensation energy for the collective state. In contrast, in conventional descriptions of superconductivity and ferromagnetism the transitions to these collective states result in *increase* in kinetic energy of the carriers and are driven by lowering of potential energy and exchange energy respectively.

Key words: Quasiparticle, Dressing, Undressing, Quasiparticle Weight, Effective Mass, Holes, Optical Sum Rule, Dynamic Hubbard Model

1. Particles and quasiparticles

Quasiparticles are 'dressed' bare particles, and they have a smaller quasiparticle weight and a larger effective mass than bare particles. In several superconductors and ferromagnets of current interest there is experimental evidence that quasiparticles 'undress', and resemble more free particles, when correlations build up and the system orders. Associated with this, that the kinetic energy, that is supposed to be optimal in the Fermi liquid normal state, decreases rather than increases in the ordered state. This behavior is counterintuitive, since in a normal Fermi liquid description it is expected that quasiparticles should become further dressed and less like

free particles when they develop the correlations leading to the collective state, and that they should *pay*, rather than *gain*, kinetic energy. Several 'unconventional' theories have been proposed to explain these phenomena. Instead we propose here that in fact quasiparticle undressing is a unifying concept that can describe these collective effect in *both* new and conventional materials. The only difference is that only in the newer materials is the 'undressing phenomenology' strong enough that it is easily seen in experiments.

2. Dressing and undressing

The single particle Green's function for an electron in an electronic energy band is

$$G(k, \omega) = \frac{1}{\omega - \epsilon_k - \Sigma(k, \omega)} \quad (1)$$

Expanding the self-energy $\Sigma(k, \omega)$ around $\omega = 0$

$$\Sigma(k, \omega) = \Sigma(k, 0) + \omega \frac{\partial \Sigma}{\partial \omega} \quad (2)$$

the Green's function can be written as

$$G(k, \omega) = \frac{z_k}{\omega - \tilde{\epsilon}_k} + G'(k, \omega) \quad (3)$$

where the first term is the quasiparticle part and the second term is the incoherent part, and the 'quasiparticle weight' z_k is given by

$$z_k = [1 - \partial \Sigma / \partial \omega]^{-1} \quad (4)$$

If the momentum dependence of the self-energy can be neglected,

$$\Sigma(k, \omega) \sim \Sigma(\omega) \quad (5)$$

then we have simply $z_k = z$ and $\tilde{\epsilon}_k = z\epsilon_k$ which implies that the quasiparticle weight and effective mass m^* are simply related by

$$\frac{m}{m^*} = z \quad (6)$$

hence a highly dressed particle will have a small quasiparticle weight and a large effective mass. For the models of interest in this paper the 'local approximation' Eq. (5) is reasonable. Finally, the 'kinetic energy' of the system is defined by

$$E_{kin} = \sum_k n_k \epsilon_k \quad (7)$$

where the occupation number n_k is obtained from the single particle Green's function

$$n_k = \int_{-\infty}^{\infty} d\omega f(\omega) \left(-\frac{1}{\pi} \text{Im}G(k, \omega)\right) \quad (8)$$

with f the Fermi function. The discontinuity of n_k at the Fermi surface is the quasiparticle weight z_k . If z_k was to increase for example as the temperature is lowered, Eq. (7) predicts that the kinetic energy of the system would decrease. The existence of this general relation between quasiparticle weight increase and kinetic energy lowering was pointed out by Norman et al (1).

In the presence of interactions bare particles become dressed with quasiparticle weight z and effective mass $m^* \sim 1/z$. The residual weak interactions between these quasiparticles may cause the system to undergo a transition to a collective state. In this paper we discuss a description of superconductivity and ferromagnetism that predicts that when the collective state develops quasiparticles undress, namely, that z increases and m^* decreases. The resulting kinetic energy lowering provides the condensation energy stabilizing the ordered state.

3. Low energy effective Hamiltonians

The low energy effective Hamiltonians in our theory can be derived from the single band generalized Hubbard model

$$H = - \sum_{\langle ij \rangle \sigma} t_{ij} (c_{i\sigma}^\dagger c_{j\sigma} + h.c.) + \sum_{ijkl\sigma\sigma'} (ij|1/r|kl) c_{i\sigma}^\dagger c_{j\sigma'}^\dagger c_{l\sigma'} c_{k\sigma} \quad (9)$$

where $(ij|1/r|kl)$ are matrix elements of the Coulomb interaction involving Wannier orbitals at sites i, j, k, l . Keeping only two center integrals, we have shown that the off-diagonal interactions $(ii|1/r|ij) \equiv (\Delta t)_{ij}$ and $(ij|1/r|ji) = (ii|1/r|jj) \equiv J_{ij}$ lead to simple descriptions of superconductivity (2) and ferromagnetism (3) respectively, that have many features in common with the phenomena seen in real materials. It should be pointed out however that these off-diagonal interactions are not simply calculable by computing matrix elements of the Coulomb interaction between *fixed* Wannier orbitals (4).

The Hamiltonian that gives rise to (hole) superconductivity is

$$H_{sc} = H_{exHub} + \sum_{\langle ij \rangle \sigma} (\Delta t)_{ij} (n_{i,-\sigma} + n_{j,-\sigma}) [c_{i\sigma}^\dagger c_{j\sigma} + h.c.] \quad (10)$$

and the one giving rise to ferromagnetism is

$$H_{fm} = H_{exHub} + \frac{1}{2} \sum_{\langle ij \rangle} J_{ij} \left[\sum_{\sigma} (c_{i\sigma}^\dagger c_{j\sigma} + h.c.) \right]^2 \quad (11)$$

The 'extended Hubbard' Hamiltonian H_{exHub} includes the kinetic energy in Eq. (9) and the ordinary density-density Coulomb interactions $U = (ii|1/r|ii)$, $V_{ij} = (ij|1/r|ij)$. The 'bond charge repulsion' term in Eq. (11) describes both exchange and pair hopping processes (3), arising from the matrix elements $(ij|1/r|ji)$ and $(ii|1/r|jj)$ respectively.

These 'off-diagonal' interactions lead to a decrease of the effective mass and associated with it a decrease in the kinetic energy as the collective states develop. For ferromagnetism, the effective hopping for a carrier of spin σ is

$$t_{ij}^{eff} = t_{ij} - J_{ij} \langle c_{i,-\sigma}^\dagger c_{j,-\sigma} + h.c. \rangle \quad (12)$$

and it increases when spin polarization develops because the bond charge $\langle c_{i,-\sigma}^\dagger c_{j,-\sigma} \rangle$ decreases. For superconductivity the effective hopping for an electron is

$$t_{ij}^{eff} = t_{ij} - n(\Delta t)_{ij} \quad (13)$$

and it decreases monotonically as the number of electrons in the band increases. For holes instead the effective hopping amplitude is

$$t_{ij}^{eff} = t_{ij}^h + n_h(\Delta t)_{ij} \quad (14a)$$

with

$$t_{ij}^h = t_{ij} - 2(\Delta t)_{ij} \quad (14b)$$

and it increases as the hole concentration n_h increases. Because the *local* hole concentration around a given hole increases when holes pair, the effective hopping Eq. (14a) will increase when pairing occurs (6).

These Hamiltonians describe changes in the quasiparticle effective mass when the system enters the collective state, and also as function of doping in the normal state. However they do not properly describe the expected relation between effective mass and quasiparticle weight discussed in the previous section. This is most clearly seen for the effect of Δt in the normal state. According to the model Hamiltonian Eq. (10), the effective mass of a single hole in a filled band can be much larger than that of a single electron in an empty band, their ratio is

$$\frac{m_{hole}^*}{m_{electron}^*} = \frac{t}{t - 2\Delta t} \quad (15)$$

On the other hand, the quasiparticle weights for the single electron and the single hole in this single band model are simply $z_{el} = z_{hole} = 1$, hence the expected relation between quasiparticle weight and effective mass Eq. (6) is strongly violated.

In addition, the optical conductivity sum rule is violated. The integral of the optical conductivity in a tight binding model is given by

$$\int_0^\infty d\omega \sigma_1(\omega) \sim \langle -T_{kin} \rangle \quad (16)$$

(proportionality factors are omitted). For the Hamiltonian Eq. (10), the average kinetic energy for holes from the ij bond is

$$\langle T_{kin} \rangle_{ij} = -(t_{ij}^h + n_h(\Delta t)_{ij}) \langle c_{i\sigma}^\dagger c_{j\sigma} \rangle + \langle T_{kin}^a \rangle_{ij} \quad (17a)$$

$$\langle T_{kin}^a \rangle_{ij} = -(\Delta t)_{ij} [\langle c_{i,-\sigma}^\dagger c_{i\sigma}^\dagger \rangle \langle c_{j\sigma} c_{i,-\sigma} \rangle + \langle c_{j,-\sigma}^\dagger c_{i\sigma}^\dagger \rangle \langle c_{j\sigma} c_{j,-\sigma} \rangle] \quad (17b)$$

and it decreases below T_c as the anomalous expectation values in Eq. 17(b) become nonzero. Hence the integrated optical spectral weight (left side of Eq. (16)) increases. A similar situation occurs for ferromagnetism. However, in a real system the total optical spectral weight is conserved (optical sum rule), hence the optical sum rule is 'violated' if kinetic energy lowering occurs. The resolution of both this violation and the unphysical relation between m^* and z arises from consideration of other degrees of freedom not contained in the effective Hamiltonian Eq. (9).

4. Relation between particle and quasiparticle operators

The low energy effective Hamiltonian Eq. (9) should be understood as describing the dynamics of quasiparticles rather than bare particles. For the description of superconductivity (5) the quasiparticle operator (which we denote by $\tilde{c}_{i\sigma}$) is related to the *coherent part* of the bare particle operator $c_{i\sigma}$ by

$$c_{i\sigma} = [1 - (1 - S)\tilde{n}_{i,-\sigma}]\tilde{c}_{i\sigma} \quad (18a)$$

with $0 < S \leq 1$. Here, $c_{i\sigma}$ is an *electron* operator. The corresponding relation for *hole* operators is

$$c_{i\sigma} = S[1 + \Upsilon\tilde{n}_{i,-\sigma}]\tilde{c}_{i\sigma} \quad (18b)$$

$$\Upsilon = \frac{1}{S} - 1 \quad (19)$$

In the kinetic energy operator for bare electrons,

$$H_{kin} = - \sum_{\langle ij \rangle \sigma} t_{ij} [c_{i\sigma}^\dagger c_{j\sigma} + h.c.] \quad (20)$$

upon replacement of the bare electron operator in terms of the quasiparticle operators using Eq. (18), a 'correlated hopping' term of the form Eq. (10) results. Hence we can identify the correlated hopping amplitude as

$$(\Delta t)_{ij} = t_{ij} S(1 - S) = t_{ij}^h \Upsilon \quad (21)$$

The quasiparticle weight for holes in a filled band is $z_h = S^2$. When z_h is small, holes are heavily dressed in the normal state low hole concentration regime, and the 'undressing parameter' Υ is large. When the hole

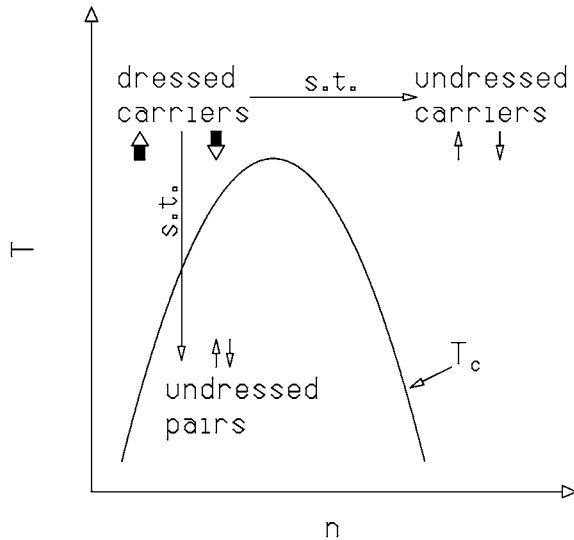


Figure 1. Undressing phenomenology in the cuprates. Both when hole carriers pair and when the hole concentration increases by doping, there is an increase in the *local* hole density around a given carrier that gives rise to undressing. This is accompanied by spectral weight transfer from high to low frequencies

concentration n_h increases, the quasiparticle weight and the quasiparticle bandwidth increase according to the relations

$$z = z_h \left(1 + \Upsilon \frac{n_h}{2}\right)^2 \quad (22a)$$

$$D = D_h \left(1 + \Upsilon \frac{n_h}{2}\right)^2. \quad (22b)$$

As a consequence, the system becomes increasingly more coherent as the hole concentration increases.

The relation between bare particle and quasiparticle operator Eq. (18) gives rise to hole superconductivity when the parameter Υ is large, as well as to the 'undressing' phenomenology observed in experiments whereby quasiparticles undress both when the temperature decreases and the system becomes superconducting and when the hole concentration is increased in the normal state. This behavior qualitatively shown in Figure 1 was predicted (7) based on microscopic considerations for the cuprates well before it was observed experimentally.

For ferromagnetism, a parallel analysis results when in the relation between bare and quasiparticle operators Eq. (18a) the site charge $n_{i\sigma}$ is replaced by the *bond* charge. Replacement in the kinetic energy Eq. (20) gives rise to exchange and pair hopping terms that give rise to ferromagnetism and to undressing (increase in quasiparticle weight and decrease in quasiparticle mass) as the system develops spin polarization (8).

5. Dynamic Hubbard models

That the conventional single band Hubbard model is fundamentally flawed is seen as follows: in the Hubbard model, destruction of an electron in a doubly occupied orbital yields the single electron state, ie

$$c_{i\sigma}|\uparrow\downarrow\rangle = |-\sigma\rangle \quad (23)$$

This relation implies that the doubly occupied state $|\uparrow\downarrow\rangle$ is a single Slater determinant. The very fact that electrons interact makes this an incorrect assumption. Hence the conventional Hubbard model fails to describe the most basic aspect of the electronic correlation problem it purports to embody, namely correlation of electrons in the same Wannier orbital.

Recognition of the fact that the doubly occupied orbital $|\uparrow\downarrow\rangle$ is a correlated state rather than a single Slater determinant leads to dynamic Hubbard models (9). The correct form of Eq. (23) is

$$c_{i\sigma}|\uparrow\downarrow\rangle = |-\sigma\rangle S + \sum_{n>0} |-\sigma>_n S_n \quad (24)$$

where $|-\sigma>_n$ are excited state of the singly occupied orbital, and $|-\sigma>\equiv |-\sigma>_{n=0}$ the ground state. Because electrons interact, S in Eq. (24) is *never* unity, and the second term on the right side of Eq. (24) is *never* zero. This leads to the relation between bare particle and quasiparticle operators Eq. (18).

We have discussed various realizations of dynamic Hubbard models, involving either an auxiliary boson degree of freedom at each site or more than one orbital per site (10). A new energy scale enters, given by the excitation energies of the states $|-\sigma>_n$. This is the energy range from which the high frequency spectral weight gets transferred from. In dynamic Hubbard models the Hubbard U becomes a dynamical variable, which can take more than one value depending on the relative state of the two electrons in the correlated state $|\uparrow\downarrow\rangle$, and destruction of an electron in that correlated state *never* yields the singly occupied state $|\sigma\rangle$ with its full amplitude. The study of dynamic Hubbard models is only in its beginning stages but it is clear already that they exhibit very rich physics absent in the conventional Hubbard model.

6. Conclusions and summary

We are proposing that there is a single unifying concept behind the two most common collective effects in metals, superconductivity and ferromagnetism: *quasiparticle undressing*. Our proposal rests on four pillars, namely: (1)

Theoretical consistency, (2) Experimental evidence, (3) Microscopic justification, (4) Philosophical considerations. We summarize arguments in each category in the following.

(1) Theoretical consistency

The theory is based on the relation between bare particle and quasiparticle operators,

$$c_{i\sigma}^\dagger = [1 - (1 - S)\tilde{n}_{local}] \tilde{c}_{i\sigma}^\dagger + \textit{incoherent part} \quad (25)$$

with $S < 1$. For the description of superconductivity and ferromagnetism \tilde{n}_{local} is the site charge or the bond charge respectively (normalized to unity). This relation gives rise to low energy effective Hamiltonians with off-diagonal interaction terms Δt and J which drive hole superconductivity and ferromagnetism respectively. Inclusion of both the local site and bond charge in Eq. (25) will yield a description of both instabilities and their competition with the same Hamiltonian.

As the collective state develops, the term \tilde{n}_{local} in Eq. (25) decreases: for ferromagnetism, spin polarization reduces the bond charge density, and for superconductivity hole pairing reduces the electronic site charge density. As a consequence the coefficient of $\tilde{c}_{i\sigma}^\dagger$ in the first term of Eq. (25) increases, and the incoherent part correspondingly decreases. This leads to an increase in the quasiparticle weight and a decrease in the quasiparticle mass, as well as lowering of kinetic energy. Spectral weight in the optical conductivity is transferred to low frequencies from the high frequency processes giving rise to the incoherent terms in Eq. (25). This framework then maintains the simple relation between quasiparticle weight and quasiparticle mass expected on general grounds, as well as explains the optical sum rule violation that occurs if only the low energy effective Hamiltonians are considered. These low energy effective Hamiltonians are seen to give rise to ferromagnetism and superconductivity both within mean field theory as well as in exact treatments.

For superconductivity, the theory predicts that it cannot occur when only electron carriers exist at the Fermi energy, because electron carriers are already undressed and will not undress further by pairing. It can only occur when hole carriers exist at the Fermi energy because holes are dressed. When the local hole concentration increases either by pairing or by hole doping in the normal state, holes undress and turn into electrons. Pairing of holes is especially favored when holes propagate in negatively charged structures, since in that case the dressing of the hole is highest and the undressing associated with hole pairing is strongest (4, 9).

(2) Experimental evidence

Certain ferromagnets exhibit clear evidence of undressing in optical spectroscopy: manganites (11), EuB_6 (12), $TlMn_2O_7$ (13), and some ferromagnetic semiconductors (14). Furthermore the anomalous lowering of resistivity below T_c and the negative magnetoresistance observed in all ferromagnets may be interpreted as originating in lowering of effective mass upon spin polarization. The undressing in optical spectroscopy may be too weak in certain metallic ferromagnets to be directly observed. The undressing has not yet been seen in photoemission experiments in the manganites, but we expect that it will be seen in the future. The reduction in the bond charge density associated with spin polarization that the theory requires (see the previous subsection) manifests itself in the anomalous thermal expansion behavior of ferromagnets below T_c (15).

High T_c cuprates exhibit abundant experimental evidence that quasiparticles undress when they pair, in photoemission (16) and optical spectroscopy (17, 18). Furthermore, optical (19) and photoemission (20) spectroscopy as well as transport (21) show that holes undress in the normal state when the hole concentration increases by doping. The fact that by pairing dressed holes turn into undressed electrons is seen directly in experiments in both conventional as well as high T_c superconductors (22, 23, 24). The fact that superconductors are frequently prone to lattice instabilities is naturally explained by the fact that many *antibonding* electronic states need to be occupied in order for the charge carriers to be hole-like. The observed isotope effects and phonon signatures in tunneling are expected to result from the fact that ionic displacements will affect the magnitude of the interaction Δt that drives superconductivity. The empirical observation that superconductors have hole carriers in the normal state was made by Chapnik (25).

(3) Microscopic justification

Analysis of the physics of electrons in atomic orbitals shows that the basic relation Eq. (18) is valid, with the parameter S decreasing as the net ionic charge Z decreases (9). Also, first principles calculation of hopping amplitudes in simple diatomic molecules show that indeed the hopping amplitude for holes is smaller than the one for electrons in certain parameter ranges (4). The effect becomes large for small interatomic distance and small Z , as expected. For ferromagnetism, first principles calculations of the relevant quantities have not yet been reported.

(4) Philosophical considerations

According to the philosophical principle known as Occam's razor, 'plurality non est ponenda sine necessitas', plurality is not to be assumed without necessity. If a single principle can explain a variety of observations it

should be preferred over multiple explanations. The principle of undressing provides a single explanation for phenomena for which a very large number of different explanations have been proposed, hence it should be preferred over the other explanations unless clearly proven wrong.

Another requirement on scientific theories is that they can be falsified by experiment. The present theory offers plenty of opportunity for falsification. A few examples of possible observations that would disprove the theory are: finding of a single superconductor that does not have hole carriers at the Fermi energy; observation of transfer of spectral weight in one or two-particle spectral functions from *low* to *high* frequencies as the collective state (superconductor or ferromagnet) develops; finding that in manganites the observed effective mass reduction is *not* accompanied by a substantially enhanced quasiparticle peak in photoemission; finding that the gap slope in superconductors does not have universal sign (2); etc.

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