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Spirals and spin bags: A link between the weak- and the strong-coupling limits of the Hubbard model

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We reconsider some of the previous studies of the interactions between the holes and the spin background in the Hubbard model in the small-doping limit. We show that the hole-hole interaction due to the transverse magnetization fluctuations (i.e., spin waves) is finite at arbitrarily small hole density. It may be comparable to the coupling due to the longitudinal magnetization fluctuations (which are the essence of the "spin-bag" mechanism of Schrieffer, Wen, and Zhang). This suggests that the two couplings should be considered simultaneously when studying the phase diagram of the lightly doped quantum antiferromagnets at the values of U/t relevant to the high-T_c superconducting materials. We also show that in the large-(U/t) limit the Hubbard-model expressions for the coupling of holes reduce to those given by Shraiman and Siggia for the t-J model. This provides a link between the weak- and the strong-coupling theories of the *doped* quantum antiferromagnets, in the small-doping limit.

Ever since the discovery of the high-T_c superconductors,[1] there has been a considerable interest in the properties of the two-dimensional (2D) doped quantum antiferromagnets[2] (AFM). While the ultimate goal remains the understanding of the AFM at relatively high doping levels ($\sim 15\%$), it has so far proven elusive. One limit where there had been some progress (at least from a theoretician's point of view) is that of a very low doping, including the studies of a single hole,[3-8] the interaction of just two holes in an otherwise ordered AFM background,[9-12] as well as the possible phase diagram[13,14] and pairing schemes[11,12,15] in the low-doping limit. These studies had been done with the t-J model,[3-7,12-14] as well as with the finite-U Hubbard model[8-11,15] (and their two-band generalizations).

Working from the t-J model, Shraiman and Siggia (SS) demonstrated that a single hole couples to the transverse (i.e., spin-wave) degrees of freedom in an AFM in a way that induces a long-range dipolar twist of the spin background.[6] In the presence of a (small) finite density of holes, a strong possibility exists that these twists arrange themselves in a pattern that leads to a spiral distortion of the spin background.[13]

In the Hubbard model, at finite U/t values, the hole also couples to the longitudinal magnetization fluctuations of the AFM background. Schrieffer, Wen, and Zhang (SWZ) considered the consequences of that coupling at low-doping levels.[11] Their "spin bag" is essentially a quasiparticle made of a hole dressed by such magnetization fluctuations. They considered the interaction between two holes caused by these fluctuations, and studied the possible pairing schemes due to this coupling.

In the spin-bag picture only the magnitude of the magnetization, and not its direction, is affected by the hole, and thus nothing like a spiral phase of SS can arise. This means that the two solutions are quite distinct from each other. However, we expect the large-U Hubbard model to behave essentially like the t-J model, and it is especially important to understand the relation between the weak- and the strong-coupling calculations when they seem to lead to such different results.

In this work, following largely the random-phase-approximation (RPA) formalism employed by SWZ, we demonstrate that the hole-hole couplings both due to the longitudinal and the transverse spin fluctuations are present and finite at arbitrarily low hole density. As a result, SWZ and SS results should be generalized by including both couplings together, raising the possibility of a more interesting phase diagram than each would produce individually.

The Hubbard model is given by the Hamiltonian

$$H=-t\sum_{\substack{\langle ij\rangle,\\ \sigma}}(c_{i,\sigma}^{\dagger}c_{j,\sigma}+\text{H.c.})+U\sum_i n_{i\uparrow}n_{i\downarrow} \ . \qquad (1)$$

The large-(U/t) limit of this model is believed to be essentially described by the t-J model,

$$H=-t\sum_{\substack{\langle ij\rangle,\\ \sigma}}(c_{i\sigma}^{\dagger}c_{j,\sigma}+\text{H.c.})+J\sum_{\langle ij\rangle}\mathbf{S}_i\cdot\mathbf{S}_j \ , \qquad (2)$$

where $J\simeq 4t^2/U$. At half-filling, it reduces to a Heisenberg model, for which the spin waves provide a rather good description of the collective modes. SWZ observed that the large-U limit of a simple RPA approximation for the transverse spin response function in the Hubbard model, gives the correct spin-wave velocity. A one-loop correction to self-energy also reproduced the spin-wave result for the reduction of the order parameter due to the quantum fluctuations.[11] This was somewhat surprising, since it was contrary to the intuitive expectation that the RPA approach should only work in the small-U limit. To see what happens away from half-filling, we inquire if the RPA expressions for the hole-hole interactions reduce, in the large-U limit, to those found by the Schwinger-boson-spinless-fermion decoupling of the electron operators in the t-J model.[12,14] We show below that this indeed occurs.

We first summarize the relevant formulas from SWZ (see Ref. 11). At half-filling, the mean-field (MF) solution with a spin density wave is given by diagonalizing,

$$H_{\rm MF}=\sum_{k,\sigma}\varepsilon_k c^\dagger_{k\sigma}c_{k\sigma}-US\sum_k[c^\dagger_{k+Q,\uparrow}c_{k\uparrow}-c^\dagger_{k+Q,\downarrow}c_{k\downarrow}]\ , \quad (3)$$

where the "free-electron" energy is given by

$$\varepsilon_k=-2t(\cos k_x+\cos k_y)\ ,$$

the nesting wave vector $Q=(\pi,\pi)$, and S is a parameter to be determined self-consistently. $H_{\rm MF}$ is solved by a linear transformation

$$\gamma^c_{k\alpha}=u_k c_{k\alpha}-v_k\sigma^3_{\alpha\beta}c_{k+Q,\beta}\ ,$$
$$\gamma^v_{k\alpha}=v_k c_{k\alpha}+u_k\sigma^3_{\alpha\beta}c_{k+Q,\beta}\ . \quad (4)$$

The resulting vacuum is given by $\gamma^c|0\rangle=\gamma^{v\dagger}|0\rangle=0$, and the diagonalized Hamiltonian is

$$H_{\rm MF}=\sum_{k,\sigma}{}'E_k[\gamma^{c\dagger}_{k\sigma}\gamma^c_{k\sigma}-\gamma^{v\dagger}_{k\sigma}\gamma^v_{k\sigma}]\ , \quad (5)$$

where the wave vectors are restricted to the magnetic Brillouin zone. In these formulas, the one-particle energies are, $E_k=(\Delta^2+\varepsilon_k^2)^{1/2}$, the rotation coefficients are

$$u_k=\frac{1}{2}\left[1+\frac{\varepsilon_k}{E_k}\right],\quad v_k=\frac{1}{2}\left[1-\frac{\varepsilon_k}{E_k}\right]\ , \quad (6)$$

and the gap parameter $\Delta=US$ is found from the usual gap equation,

$$\frac{1}{N}\sum_k{}'\frac{1}{(\varepsilon_k^2+\Delta^2)^{1/2}}=\frac{1}{U}\ .$$

SWZ studied the charge, the longitudinal spin, and the transverse spin fluctuations around the spin density wave ground state, and the interactions between holes mediated by these fluctuations. Of interest to us is the effective Hamiltonian $H=H_z+H_{+-}$ due to the two-spin fluctuation channels, where

$$H_z=-\frac{1}{4N}\sum_{kk'q}\sum_{\substack{\alpha\beta\\ \alpha'\beta'}}V_z(k-k')\sigma^3_{\alpha'\alpha}\sigma^3_{\beta'\beta}c^\dagger_{k'\alpha'}c^\dagger_{-k'+q,\beta'}c_{-k+q,\beta}c_{k\alpha}\ , \quad (7)$$

$$H_{+-}=-\frac{1}{N}\sum_{kk'q}\sum_{\substack{\alpha\beta\\ \alpha'\beta'}}V_{+-}(k-k')\sigma^+_{\alpha'\alpha}\sigma^-_{\beta'\beta}c^\dagger_{k'\alpha'}c^\dagger_{-k'+q,\beta'}c_{-k+q,\beta}c_{k\alpha}\ . \quad (8)$$

In the RPA approximation,

$$V_z(q)=\frac{U^2\chi_0^{zz}(q)}{1-U\chi_0^{zz}(q)},\quad V_{+-}(q)=\frac{U^2\chi_0^{+-}(q)}{1-U\chi_0^{+-}(q)}\ . \quad (9)$$

Here, χ_0 are the "noninteracting" response functions at $\omega=0$, given by

$$\chi_0^{zz}(q)=\frac{1}{N}\sum_k{}'\left[1-\frac{\varepsilon_k\varepsilon_{k+q}+\Delta^2}{E_kE_{k+q}}\right]\left[\frac{1}{E_k+E_{k+q}}\right]\ , \quad (10)$$

$$\chi_0^{+-}(q)=\frac{1}{N}\sum_k{}'\left[1-\frac{\varepsilon_k\varepsilon_{k+q}-\Delta^2}{E_kE_{k+q}}\right]\left[\frac{1}{E_k+E_{k+q}}\right]\ . \quad (11)$$

One then rewrites this Hamiltonian in terms of the mean-field one-electron eigenstates, $\gamma^v_{k\sigma}$ and $\gamma^c_{k\sigma}$, and one further restricts it to the pairs of holes with opposite momenta in the valence band only. One obtains,

$$H_z=-\frac{1}{4N}\sum_{k,k'}{}'\sum_{\substack{\alpha\alpha'\\ \beta,\beta'}}[V_z(k-k')l^2(k,k')\sigma^3_{\alpha'\alpha}\sigma^3_{\beta'\beta}+V_z(k-k'+Q)m^2(k,k')\delta_{\alpha',\alpha}\delta_{\beta'\beta}]\times\gamma^{v\dagger}_{k'\alpha'}\gamma^{v\dagger}_{-k'\beta'}\gamma^v_{-k\beta}\gamma^v_{k\alpha}\ , \quad (12)$$

$$H_{+-}=-\frac{1}{N}\sum_{k,k'}{}'\sum_{\substack{\alpha\alpha'\\ \beta,\beta'}}[V_{+-}(k-k')n^2(k,k')-V_{+-}(k-k'+Q)p^2(k,k')]\times\sigma^+_{\alpha'\alpha}\sigma^-_{\beta'\beta}\gamma^{v\dagger}_{k'\alpha'}\gamma^{v\dagger}_{-k'\beta'}\gamma^v_{-k\beta}\gamma^v_{k\alpha}\ , \quad (13)$$

where the coherence factors are

$$m(k,k')=u_kv_{k'}+v_ku_{k'},\quad l(k,k')=u_ku_{k'}+v_kv_{k'}\ ,$$
$$p(k,k')=u_kv_{k'}-v_ku_{k'},\quad n(k,k')=u_ku_{k'}-v_kv_{k'}\ . \quad (14)$$

The mean-field energy $E_k=(\Delta^2+\varepsilon_k^2)^{1/2}$ is degenerate along the Brillouin zone boundary. This is an artifact of the mean-field approximation; it is believed that the t-J model has the band minima at $k=(\pm\pi/2,\pm\pi/2)$ for the physically interesting values of t/J. In the following we assume the same is true of the Hubbard model for the relevant U/t values.[16,17] Then, at low densities, the holes will form Fermi pockets around $k=(\pm\pi/2,\pm\pi/2)$. Note that $k=(\pi/2,\pi/2)$ is equivalent to $k=(-\pi/2,-\pi/2)$ in the magnetic Brillouin zone, and in the extended zone scheme we limit our attention to the Fermi pocket of holes near, say, $k=(\pi/2,\pi/2)$.

SWZ observed that the coherence factors $n(k,k')$ and $p(k,k')$ which are present in the H_{+-} channel are very nearly zero when both k and k' are near the Brillouin zone boundary, since in that case $u_k\sim v_k\sim 1/\sqrt{2}$. At a low-hole density, when the Fermi pockets are small, these factors are very nearly zero for the scattering processes between the various parts of the Fermi surface. On the contrary, factors $m(k,k')$, $l(k,k')$ which are present in the H_z channel are close to unity. Thus SWZ focused on the consequences of the H_z interaction, which is the crucial ingredient in their "spin-bag" approach to doped

AFM.

The main thesis of this note is that H_{+-} is also finite, despite the vanishingly small coherence factors $p(k,k'),n(k,k')$. The key idea is that $V_{+-}(k'-k+Q)$ has a Goldstone pole at $q=(k'-k)\to 0$, and this pole cancels the zero in $p^2(k,k')$. To demonstrate this, consider,

$$p^2(k,k')=(u_k v_{k'}-u_{k'}v_k)^2 = \frac{1}{4}\left[\left[1+\frac{\varepsilon_k}{E_k}\right]^{1/2}\left[1-\frac{\varepsilon_{k'}}{E_{k'}}\right]^{1/2} - \left[1-\frac{\varepsilon_k}{E_k}\right]^{1/2}\left[1-\frac{\varepsilon_{k'}}{E_{k'}}\right]^{1/2}\right]^2 . \quad (15)$$

When $k\to(\pi/2,\pi/2)$,

$$\varepsilon_k=-2t(\cos k_x+\cos k_y)\simeq 2t(\delta k_x+\delta k_y) , \quad (16)$$

where $\delta k_x=(k_x-\pi/2)$ and $\delta k_y=(k_y-\pi/2)$. In the same limit, $E_k\to\Delta$. Thus, when both k and k' are close to this band minimum,

$$p^2(k,k')\simeq\frac{1}{4}\left[\frac{\varepsilon_k-\varepsilon_{k'}}{\Delta}\right]^2\simeq\frac{t^2}{\Delta^2}(q_x+q_y)^2 , \quad (17)$$

where $q=k-k'$.

We now go back to $V_{+-}(q+Q)$, which in the $\omega=0$, $q\to 0$ limit had been calculated to yield,

$$V_{+-}(q+Q)=U^2\chi^{+-}_{\rm RPA}(q+Q)\simeq\frac{1}{t^2yq^2} , \quad (18)$$

where

$$y\equiv\frac{1}{N}\sum_k{}'\frac{\sin^2 k_x}{E_k^3} . \quad (19)$$

Combining Eqs. (17) and (18) for $p^2(k,k')$ and $V_{+-}(q+Q)$, and substituting into Eq. (13) for H_{+-}, we obtain our key result for the hole-hole interaction strength due to the spin waves,

$$V_{+-}(q+Q)p^2(k,\,k+q)\simeq\frac{1}{(t^2y)q^2}\,\frac{t^2}{\Delta^2}(q_x+q_y)^2 = \frac{1}{y\Delta^2}\frac{(q_x+q_y)^2}{q^2} . \quad (20)$$

Here, we have a finite interaction strength in the limit $\omega=0$, $q\to 0$, regardless of the hole density.

This interaction is of the same functional form as the one found by SS for the t-J model.[12] In the large-U limit we also get the same coupling strength as in the unrenormalized (i.e., without the vertex corrections) SS calculation. Indeed, in the $t/U\to 0$ limit we have, $y\to 1/(4\Delta^3)$ and $\Delta\to U/2$, and we obtain from Eq. (20),

$$V_{+-}(q+Q)p^2(k,k+q)\simeq 2U\frac{(q_x+q_y)^2}{q^2} . \quad (21)$$

SS obtained the following Hamiltonian,

$$H=\frac{1}{N}\sum_{k,k',q}{}'\,V(k,k',q)\bar\psi_k^A\psi_{k+q}^B\bar\psi_{k'+q}^B\psi_{k'}^A , \quad (22)$$

where (before the vertex corrections),

$$V(k,k',q)=-\frac{8t^2}{J}\left[\frac{(\lambda_k-\lambda_{k+q})(\lambda_{k'}-\lambda_{k'+q})}{1-\lambda_q}+\frac{(\lambda_k+\lambda_{k+q})(\lambda_{k'}+\lambda_{k'+q})}{1+\lambda_q}\right] , \quad (23)$$

in which

$$\lambda_k=\tfrac{1}{2}(\cos k_x+\cos k_y) .$$

It is easy to check that when $k,k'\to(\pi/2,\pi/2),q\to 0$, we obtain,

$$V(k,k',q)\simeq-\frac{8t^2}{J}\frac{(q_x+q_y)^2}{q^2} . \quad (24)$$

The large-U limit of the Hubbard model corresponds to $J=4t^2/U$ in the t-J model, and thus both the coefficients and the functional forms in Eqs. (21) and (24) are the same. We know that the RPA correctly reproduces the spin-wave results in the large-U limit at half-filling.[11] Thus the fact that the hole-hole interaction came out the same as well demonstrates that the (bare) vertex is identical to that obtained by the Schwinger-boson–slave-fermion decoupling of the electron operators in the t-J model.[3,6] This establishes a definitive connection between the "weak-coupling" approach of SWZ and the t-J model calculations by SS and others. In particular, all of SS calculations regarding the possibility of a spiral phase can now be repeated for a weak-coupling case.

One would like to compare the relative magnitude of H_z and H_{+-} at the realistic values of U/t. Unfortunately, the RPA expressions can be poor guides because of the vertex corrections. The most extreme example is offered by Eq. (21) for the strength of H_{+-} in the large-(U/t) limit. It is clearly unphysical, as the coupling strength should not grow indefinitely with U. In the t-J model language, Eq. (24) is unphysical when $t/J\gg 1$. In fact, SS argued that the coupling constant $\sim t^2/J$ should renormalize to $\sim J$ in that limit. This would correspond to the coefficient $2U$ in Eq. (21) being renormalized into one of order t^2/U at large U/t. In that limit, $V_z(q)$ given in Eq. (9), leads to $V_z(Q)\sim 16t^2/U$. We do not know at present how this gets renormalized due to the vertex corrections. Thus we cannot draw any conclusions about the relative strength of H_z and H_{+-} in the large U/t limit. We do expect the importance of the vertex corrections to diminish at small U/t values, and the results of calculating the coupling strengths from Eqs. (9),(10), (19) and (20) for several representative U/t values are as follows: for $t=1$, $U=2.28$, we have $\Delta=0.5$ and,

$$V_{+-}(q+Q)p^2(k,\,k+q)\to 10.3\frac{(q_x+q_y)^2}{q^2} , \qquad V_z(q+Q)m^2(k,\,k+q)\to 2.45 ; \quad (25)$$

when $t=1$, $U=3.29$, we have $\Delta=1.0$, and we obtain

$$V_{+-}(q+Q)p^2(k,\,k+q)\to 11.3\frac{(q_x+q_y)^2}{q^2} , \qquad V_z(q+Q)m^2(k,\,k+q)\to 2.41 . \quad (26)$$

Even at these smaller U/t values, unless we calculate the vertex corrections, these numbers are at best suggestive of H_z and H_{+-} being comparable in strength.

To see if the two interactions together may behave differently than each would separately, we look more closely at their functional forms. H_z is a short-range interaction with an attractive spin-independent dominant term. It also has a spin-dependent term $\sim\sigma_1^z\sigma_2^z$, which is attractive in the spin-symmetric channel, and repulsive in the spin-antisymmetric channel [cf. Eq. (12)]. The spin dependence of H_{+-} is $\sim(\sigma_1^+\sigma_2^- + \sigma_1^-\sigma_2^+)$. Upon taking a Fourier transform of $V(q)\sim(q_x+q_y)^2/q^2$, we obtain in coordinate space,

$$H_{+-}(\mathbf{r})\sim-\left[\delta(\mathbf{r})+\frac{1}{2\pi}\frac{2xy}{r^4}\right](\sigma_1^+\sigma_2^- + \sigma_1^-\sigma_2^+) . \quad (27)$$

Due to a finite momentum cutoff, the delta function is simply a short-range interaction, which is attractive in the spin-symmetric channel and repulsive in the spin-antisymmetric one. The second term is a long-range dipolar interaction, and similarly to its three-dimensional analogue, it is repulsive or attractive depending on the instantaneous relative location of the two holes.

The spiral phase proposed by SS is due to the alignment of spins by the short-range (i.e., the contact) term in Eq. (27). The fact that the holes are also coupled to the long-range distortions of the spin background then leads to a spiral twist of the background. It is essential for the spiral that the spins be aligned in the plane perpendicular to the Néel axis. Should the strength of the spin-dependent term in H_z exceed that of the H_{+-} (for example, at lower-U values), the spins will align along the Néel axis, and the spiral will disappear. The possibility of this transition clearly deserves further study.

As another illustration of how the two interaction terms may play against each other, consider the superconducting gap equation. SWZ showed that H_x alone leads to the pairing in the usual spin-antisymmetric channel. Assuming that the angularly-dependent long-range term in H_{+-} averages to zero, we observe that the short-range term will be repulsive in the spin-antisymmetric channel. Thus, if the strength of H_{+-} is sufficiently large, the pairing produced by H_z will be entirely suppressed.

There is a simple intuitive picture that clarifies this result. It is known that in the magnetically disordered phase, the paramagnetic fluctuations depress the superconducting transition temperature in the spin-singlet channel.[18] A qualitatively similar phenomenon can be seen to occur here. Both the spin-dependent piece of H_z [cf. Eq. (12)] and the whole of H_{+-} are repulsive in the spin-antisymmetric channel. In the rotationally-invariant case, H_{+-} would be equal to the sum of the spin-dependent parts of H_z and the charge-fluctuation part of the total Hamiltonian. This equality is generally no longer true in the spin-ordered state, due to the presence of the broken symmetry. One should also add that the frequency cutoffs in H_z and H_{+-} will also be different in the presence of the broken symmetry.

In conclusion, we have offered evidence that both the spin bag and the spiral phase ideas are relevant to understanding the low-hole-density behavior of the Hubbard model at the realistic values of U/t. We did this by demonstrating analytically that the interaction term that had been used[12,13] to derive a spiral phase in the context of the *t-J* model, is already present in the RPA weak-coupling calculations on the Hubbard model, regardless of the hole density.

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