Spontaneous spin stripe dimerization in the doped t-J model.

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To investigate spin dimerization in the t–J model we consider the extended t–J = δ model with explicit spin dimerization introduced via parameter δ. At zero doping the dimerized spin liquid is unstable at δ ≤ δc ≈ 0.3. We demonstrate that the doping stabilizes the dimerized stripe phase: the δc(x) decreases when doping x increases. At doping larger than critical, x > x_c, the dimerized phase is stable even without explicit dimerization, i.e. at δ = 0.

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It is widely believed that the 2D t–J model is relevant to the low energy physics of high-temperature superconductors. This is why investigation of this model is of great interest both for theory and experiment. In spite of great efforts during more than a decade there is no full understanding of the phase diagram of the t–J model, however some facts are well established. At zero doping the model is equivalent to the Heisenberg model on a square lattice which has long range Neel order. It was first formulated by Read and Sachdev and was then analyzed Hubbard-Heisenberg model in the weak-coupling regime. Grilli, Castellani and G. Kotliar considered SU(N), N → ∞, t–J model, and very recently Vojta and Sachdev considered Sp(2N), N → ∞, t–J model with long range Coulomb interaction. These works indicated a stability of the spin-dimerized phase in some region of parameters, providing a very important guiding line. However relevance of these results to "physical regime" of the t–J model remained unclear. In the present work we demonstrate that the spin-dimer order is stable, the only small parameter used in the analysis is hole concentration with respect to the half filling.

The Hamiltonian under consideration is

\[ H = -t \sum_{\langle ij \rangle} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{\langle ij \rangle} J_{ij} \left( S_i S_j - \frac{1}{4} n_i n_j \right). \]  

(1)

\( c_{i\sigma}^\dagger \) is the creation operator of an electron with spin \( \sigma \) \((\sigma = \uparrow, \downarrow)\) at site \( i \) of the two-dimensional square lattice. The \( c_{i\sigma}^\dagger \) operators act in the Hilbert space with no double electron occupancy. The \( \langle ij \rangle \) represents nearest neighbour sites. The spin operator is \( S_i = \frac{1}{2} \sum_{\alpha, \beta} c_{i\alpha}^\dagger c_{i\beta} \sigma_{\alpha\beta} \), and the number density operator is \( n_i = \sum_{\sigma} c_{i\sigma}^\dagger c_{i\sigma} \). Antiferromagnetic interactions \( J_{ij} > 0 \) are arranged in a stripe pattern shown in Fig. 1: solid links correspond to \( J_{ij} = 1 \), and dashed links correspond to \( J_{ij} = J(1 - \delta) \). At half filling \( \langle n_i \rangle = 1 \) the Hamiltonian has already been studied for \( \delta > \delta_c \approx 0.303 \) the ground state is a quantum disordered state with gapped spectrum, and for \( \delta < \delta_c \) there is spontaneous Neel ordering with gapless spin waves.

In order to study the stability of the dimer phase we first derive an effective Hamiltonian in terms of bosonic operators creating spin-wave triplets (magnons) \( t_{i\alpha}^\dagger \), \( \alpha = x, y, z \) and fermionic operators creating holes \( a_{i\uparrow}^\dagger \), \( \sigma = \uparrow, \downarrow \) from the spin singlets shown in Fig. 1. This Hamiltonian consists of four parts: the spin-wave part \( H_t \), the hole part \( H_h \), the spin-wave-hole interaction \( H_{th} \), and the hole-hole interaction \( H_{hh} \). Let us start from \( H_t \). Similar effective theories have been derived in Refs. [10] and we only present the result: \( H_t = H_2 + H_3 + H_4 + H_U \), where

\[ H_2 = \sum_{k, \alpha} \left\{ A_k a_{k, \alpha}^\dagger t_{\alpha}^\dagger a_{k, \alpha} + \frac{B_k}{2} \left( t_{-\alpha}^\dagger t_{\alpha}^\dagger - a_{\alpha}^\dagger a_{\alpha}^\dagger + \text{h.c.} \right) \right\}, \]

\[ H_3 = \sum_{1+2=3} R(k_1, k_2) e_{\alpha\beta\gamma} t_{k_1, \alpha}^\dagger t_{k_2, \beta}^\dagger t_{k_3, \gamma}^\dagger + \text{h.c.}, \text{ and } H_4 = \]
are caused by the quartic interaction "triple" interaction also some contribution to the self-energy caused by the

\[ \sum_{1+2=3+4} T(k_1 - k_3)(\delta_{\alpha\beta}\delta_{\gamma\delta} - \delta_{\alpha\beta}\delta_{\gamma\delta})t^{\dagger}_{k_1\alpha}\sigma_{k_2\beta}\sigma_{k_3\gamma}t_{k_4\delta}. \]

We also introduce an infinite repulsion on each site, in order to enforce the kinematic constraint

\[ t^{\dagger}_{i\alpha}t_{i\beta} = 0. \]

\[ H_U = U \sum_{i,\alpha} t^{\dagger}_{i\alpha}t_{i\beta}t_{i,\alpha}, \quad U \to \infty \]

(2)

The following definitions are used in \( H_2 \): \( B_k = j(\cos k_x - 0.5 \cos k_y) \) and \( A_k = J_\perp + B_k \). The matrix elements in the quartic and cubic interaction terms are:

\[ T(k) = j(0.25 \cos k_x + 0.5 \cos k_y) \] and \( R(p, q) = 0.25 j(\sin q_x - \sin p_x) \). Throughout the paper we work in the Brillouin zone of the dimerized lattice.

At zero doping \( \langle n_i \rangle = 1 \) \( H_k \) is an exact mapping of the original Hamiltonian \( \mathcal{H} \). To analyse this case it is enough to apply the technique \( \mathcal{H} \). The result for the normal spin-wave Green’s function reads:

\[ G_N(k, \omega) = \frac{\omega + A_k(-\omega)}{\{\omega + A_k(-\omega)\} \{\omega - A_k(\omega)\} + B_k^2} \]

(3)

where \( A_k(\omega) = A_k + \Sigma_{H}^N(k) + \Sigma_{H}^{\alpha}(k, \omega) \) and \( \tilde{A}_k(\omega) = B_k + \Sigma_{H}^{\alpha}(k) \). Normal \( \Sigma_{H}^N \) and anomalous \( \Sigma_{H}^{\alpha} \) self-energies are caused by the quartic interaction \( H_4 \) and the most important contribution \( \Sigma_{H}^{(1)} \) comes from the Brueckner diagrams as described in [17]. Strictly speaking there is also some contribution to the self-energy caused by the "triple" interaction \( H_3 \). However this contribution is very small (see, e.g. Ref. [18]) and therefore we neglect it.

Expansion of the self-energy in powers of \( \omega \) near \( \omega = 0 \) gives quasiparticle residue and spin-wave spectrum

\[ Z^{-1}(k) = 1 - \frac{\delta \Sigma_{H}^N(k)}{\omega_k}, \quad \omega_k = Z_k \sqrt{[A_k(0)]^2 - B_k^2}. \]

Expressions for effective Bogoliubov parameters \( u_k \) and \( v_k \) are given in [13]. The spin-wave gap \( \Delta = \omega_{k_0}, k_0 = (0, \pi) \), obtained as a result of a selfconsistent solution of Dyson’s equations is plotted in Fig.2 (line at \( x = 0 \)). The critical value of the explicit dimerization (point where the gap vanishes) \( \delta_c = 0.298 \) is in agreement with results of series expansions [13] and quantum Monte Carlo simulations [15]. The validity of the Brueckner approximation is justified by the smallness of the gas parameter

\[ n_t = \sum_{i\alpha} t^{\dagger}_{i\alpha}t_{i\alpha}. \]

At the critical point \( n_t = 0.13 \).

Consider now doping by holes. On the single dimer \( |s\rangle \) the hole can exist in symmetric and antisymmetric states. Because of hopping between the dimers there is mixing between these states, but the mixing is very small (few per cent) and can be neglected. The symmetric state has substantially lower energy and therefore only this state is populated at doping. The corresponding hole creation operator \( a^{\dagger} \) is defined in the following way:

\[ \sqrt{2}a^{\dagger}_{\sigma} |s\rangle = (c^{\dagger}_{k,\sigma} + c^{\dagger}_{k,\pi}) |0\rangle, \]

where 1 and 2 numerate the dimer sites. Bare hole dispersion can be found by calculating hopping matrix elements. This gives

\[ H_h = \sum \epsilon_p + const) a^{\dagger}_{p,\sigma}a_{p,\sigma}, \]

where the \( const \) is chosen in such a way that

\[ \epsilon_p = t(\cos p_y + 0.5 \cos p_x + 1.5) \]

(4)

vanishes at the minimum: \( \epsilon_{p_0} = 0, p_0 = (\pi, \pi) \).

The spin-wave-hole interaction \( H_{h\sigma} \) can be easily calculated in the way similar to that for doped spin-ladder [13][14]. This interaction consists of two parts. The first one is interaction of a hole and a magnon positioned at different dimers. This is a relatively weak interaction which can be neglected [24]. The second part, which gives the main effect, comes from the constraint that a hole and a magnon can not coexist at the same dimer:

\[ t^{\dagger}_{i\alpha}a_{\alpha\delta} = 0. \]

To deal with this constraint we introduce, similarly to (2), an infinite repulsion

\[ H_U = U \sum_{i,\alpha} t^{\dagger}_{i\alpha}t_{i\alpha}a_{\alpha\sigma}, \quad U \to \infty. \]

(5)

The exact hole-magnon scattering amplitude caused by this interaction can be found via Bethe-Salpeter equation shown in Fig.3a. It is similar to that for magnon-magnon scattering [17]. The result is

\[ \Gamma(E, k) = \frac{Z_k v_k^2}{E - \omega_k - \epsilon_{k-q}} \]

(6)

where \( E \) and \( k \) is total energy and total momentum of the incoming particles.

Let us denote the hole concentration by \( x = n/N \), where \( n \) is number of holes, and \( N \) is number of sites. Hence on-site electron occupation number is \( \langle n_i \rangle = 1 - x \). Concentration of holes in times of the dimerized lattice is two times larger \( n/(0.5N) = 2x \), and this is the gas parameter of the magnon-hole Brueckner approximation. According to [14] the holes are concentrated in the pocket in the vicinity of \( p_0 = (\pi, \pi) \). Therefore the magnon normal self-energy described by the diagram Fig. 3b is

\[ \Sigma_{H}^{(2)}(k, \omega) = 2x\Gamma(\omega, k + p_0) \]

(7)

It is instructive to consider first the case which allows an analytical solution: \( J_\perp \gg j, \sqrt{2}\pi x \ll 1 \). Bare magnon dispersion in this case is \( \omega_k \approx J_\perp + j(\cos k_x - 0.5 \cos k_y) \) and hence the integrals in [14][16] can be calculated analytically with logarithmic accuracy. This gives

\[ \Sigma_{H}^{(2)}(k, \omega) = \frac{2}{\ln(12.5/\mu)} + i\pi \theta(\delta \omega), \]

(8)

where \( \delta \omega = [\omega - \omega_{k_0} + j(\omega_k - \omega_{k_0})/(t+j)]/(t+j) \), \( \mu = \max(\delta \omega, \sqrt{2}\pi x) \), and \( \theta(\delta \omega) \) is a step function. The magnon Green’s function is \( G(k, \omega) = \omega - \omega_k - \Sigma_{H}^{(2)}(k, \omega) \) \]. For illustration the spectral function \( ImG(\omega) \) at \( k = k_0, t/j = 3 \) and different \( x \) is plotted in Fig.4. There are several conclusions from formula (8) and Fig. 4: 1) doping pushes the spin-wave spectrum up, 2) the effect is increasing with hopping \( t \), 3) finite width appears, 4) there is only a logarithmic dependence on the infrared cutoff. Let us stress the importance
of the point (4). It means that the effect is practically independent of the long-range dynamics. Moreover, near the critical point (\(\Delta = 0\)) the situation is even better: the spin-wave spectrum is linear and even the logarithmic divergence disappears. Thus in the 2D case there is separation of scales which justifies Brueckner approximation. If we tried to apply the described approach to the 1D case (say a doped spin ladder) we would get into trouble: power infrared divergence appears in Brueckner diagram and hence there is no justification for gas approximation. Let us also comment on the point (3) (width). There is a "triple" contribution to the magnon self-energy. Fig. 3c. This is a long-range contribution which is much less important than the Brueckner one, and this is why we neglect it (cf. with Ref. [10]). However this diagram influences the width of the magnon spectral function.

In the general case there are two contributions to the Brueckner self-energy: \(\Sigma^{(1)}_{\text{Br}}\), which is due to the magnon-magnon constraint, and \(\Sigma^{(2)}_{\text{Br}}\), which is due to the magnon-hole constraint. To find the spin wave spectrum one has to solve self-consistently Dyson’s equation for Green’s function \([3]\), as it is described in Ref. [17]. Results for the spin-wave "gap" \(\Delta\) as a function of explicit dimerization \(t\) for different hole concentrations \(x\) and \(t/J = 3\) are plotted in Fig. 2. Strictly speaking at \(x \neq 0\) the \(\Delta\) is not a gap because of the large decay width. What we plot is the position of the centre of gravity of the magnon spectral function. However at \(\Delta \rightarrow 0\) the width vanishes, and therefore the critical regime is uniquely defined. When \(\Delta\) is not small there is an interesting question of calculation of the exact shape of magnon spectral function. However to resolve this problem one needs to include long-range dynamics (diagram Fig.3c).

It is clear from Fig.2 that at \(t/J = 3\) and \(x > x_c \approx 0.090\) the "gap" remains finite even at \(\delta = 0\). This is regime of spontaneous dimerization. For \(t/J = 2\) the critical concentration is \(x_c = 0.106\), and for \(t/J = 1\), \(x_c = 0.132\). Thus the doping stabilizes the dimerized phase. The larger the hopping \(t\), the stronger the effect of stabilization. (The same follows from eq. [3].) This statement is true only if \(t/J \lesssim 10\). At \(t/J \sim 10\) there is a crossover to quasiparticles with higher spin (hole-magnon bound states) \([3]\) which indicate transition to the Nagaoka regime. The small parameter of the Brueckner approximation is concentration of holes in the dimerized lattice: \(2x\). Therefore at \(t/J = 3\) one should expect \(\sim 20\%\) accuracy in calculation of \(x_c\). Note that the value of \(x_c\) is close to that found in \([4]\) from the Neel state.

An important effect related to the stabilisation is suppression of spin wave quantum fluctuations by doping. At \(x = 0\) and \(\delta = \delta_c = 0.298\) the density of spin fluctuations is \(n_t \approx 0.13\). Increasing of the hole concentration to \(x = 0.1\) (at \(t/J = 3\) and \(\delta = \delta_c\)) gives \(n_t \approx 0.02\). At the critical point \(t/J = 3\), \(\delta = 0\), \(x = x_c = 0.09\) the density is just \(n_t \approx 0.07\) (see also \([21]\)).

The phase diagram of the \(t - J - \delta\) model at zero temperature is presented in Fig.5. Because of the mobile holes the dimerized spin liquid is a conducting state. Stability of this state is a very robust effect because it is due to the high energy correlations (typical energy scale \(\sim 2t\)). There are also low energy (long range) effects with typical energy scale \(\sim 2tx\) which can lead to hole-hole pairing, small amplitude density waves etc. We do not consider these effects in the present work because they are secondary with respect to the main one: spin dimerization. It is also worth noting that one can introduce additional parameters \(t'\) and \(t''\) (next and next-next neighbour hopping) which influence single hole dispersion \([11]\), shift position of the minimum and change shape of the "Fermi surface": stabilization is not sensitive to these details.

Strictly speaking one can not exclude a possibility that at decreasing \(\delta\), at some point there is a first order phase transition to an absolutely different phase. However such a transition at zero temperature always has a precursor: some specific bound state. The examples are: hole-magnon bound state for transition to Nagaoka regime in the present model at very large \(t\), multi-magnon bound states for a frustrated spin-ladder as a precursor of spinon deconfinement \([21]\), and multi-magnon bound states in 2D \(J_1 - J_2\)-model at the 1st order transition point \(J_2/J_1 \approx 0.6\) \([10]\). In the present model we do not see any hint of such precursors and therefore we conclude that the first order phase transition is highly unlikely.

We have discussed in detail the transition to the Neel state at small hole concentration \(x\). It is also clear that at large \(x\) there is a 2nd order transition to normal Fermi liquid shown schematically in Fig. 5 by the dashed line. One can say that it happens when hole concentration in the dimerized lattice is equal to unity, \(2x \sim 1\). However this is only a crude estimate. Unfortunately we can not describe this part of the diagram more precisely because our approach assumes that \(2x \ll 1\).

It has been shown recently that Heisenberg antiferromagnet on triangular lattice is very close to the instability with respect to spontaneous dimerization \([22]\). We would like to note that it is highly likely that in this model doping also stabilizes the dimerized phase.

In conclusion, using the dilute gas approximation we have analyzed the phase diagram of the \(t - J - \delta\) model and the stability of spin-dimerized phase. At doping larger than the critical one, \(x > x_c \approx 0.09\), the dimerized phase is stable even without explicit dimerization.

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FIG. 1. Stripe spin dimerization on square lattice. Solid links correspond to $J_\perp = J(1 + \delta)$, and dashed links correspond to $j = J(1 - \delta)$.

FIG. 2. The magnon "gap" (centre of gravity of spectral function) as a function of explicit dimerization $\delta$ for $t/J = 3$ and different values of hole concentration $x_i$ ($n_i = 1 - x$).

FIG. 3. (a) Bethe-Salpeter equation for hole-magnon scattering vertex $\Gamma$. Solid line corresponds to the hole and dashed line to the magnon. (b) Brueckner contribution to the magnon self energy. (c) "triple" contribution to the magnon self-energy.

FIG. 4. Magnon spectral density at $k = k_0 = (0, \pi)$ in the limit $J_{\perp} \gg j$, $t/j = 3$, and different hole concentrations.

FIG. 5. Phase diagram of the $t-J-\delta$ model ($t/J = 3$) in the plane doping ($x$) - explicit dimerization ($\delta$).
Fig. 2

![Graph showing \( \frac{\Delta}{J} \) as a function of \( \delta \) for different values of \( x \):
- \( x = 0.125 \)
- \( x = 0.1 \)
- \( x = x_c = 0.09 \)
- \( x = 0.05 \)
- \( x = 0 \).]
a) \[ \Gamma \quad = \quad \text{Fig. 3} \]
Fig. 5

Normal Fermi liquid

Dimerized spin liquid

$\chi_c = 0.090$

$\delta_c = 0.298$