PAIRING AND PSEUDOGAP IN DOPED ANTIFERROMAGNETS*

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An effective Hamiltonian representing propagation and interaction of spin polarons forming in weakly doped antiferromgnets is derived. The systems becomes superconducting upon doping. Paring may be attributed to kinetic energy saving due to a particular type of motion of a spin bipolaron, which corresponds to creep of a line consisting of defects in the antiferromagnetic spin background which connects two holes. That line moves by shrinking and expanding at opposite ends. The kinetic energy term in the Hamiltonian is effective at all stages of this process, and the term related to the magnetic exchange does not have to intervene, not like in the case of a single propagating hole, which lowers the kinetic contribution to the energy. The effective attraction is strongest in the undoped system where the antiferromagnetic order is most robust, but the superconducting order parameter vanishes when the doping parameter decreases which should be attributed to emptying the spin polaron band and approaching the Mott insulator phase. Since the normal phase representing a gas of single spin polarons is unstable toward formation of bound hole pairs a pseudogap forms in the excitation spectrum.

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Recently, a convincing justification by means of a numerical method has been provided, that the t-J model (TJM) becomes superconducting (SC) in the region of low doping [1]. The importance of this result is related to the fact that TJM may serve as a minimal model to describe doped antiferromagnets (AF) which like in the case of the cuprates reveal the phenomenon

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of high temperature superconductivity (HTSC). According to some earlier scenarios [2] underlying some analytical calculations for doped AF, superconducity is mediated in that system either by reduction of the diagonal part of the exchange energy, that corresponds to the Ising model, when two holes occupy nearest neighbor sites or by the exchange of spin waves . On the other hand, it seems that the mechanism of binding in the TJM is well understood in terms of the spin polaron (SP) and spin bipolaron (SPB) formation [3]. A lot of evidence has been accumulated, by comparing results of numerical and analytical calculations, that such a scenario is valid. As examples may serve calculations of spectral density and electron momentum distribution, optical conductivity and current correlation function which takes a form corresponding to a staggered flux phase. Stimulated by applicability of the SP approach to description of many properties which reveal weakly doped AF we shall apply that method to the analysis of the hypothetical SC state. Our calculation explicitly demonstrate that the lowering of energy, by reducing by one the number of broken bonds if two holes occupy nearest neighbor sites is ineffective because holes can not hop on top of each other and a lot of kinetic energy is lost or in other words the value of the kinetic energy is raised. In addition, it turns out that propagation of spin excitations in the form of spin waves is not relevant to pairing.

In order to be more specific we will describe now how to define formally a SP and a SBP. It seems that physics of weakly doped AF is in a straightforward way governed by two obvious but opposite tendencies to minimize the kinetic and exchange energies represented by two respective terms in the effective Hamiltonian for such a system which is the t-J model. The exchange term prefers the AF correlations which range is not necessarily infinite. Coherent hole motion should somehow adjust to the local spin arrangement. If, for simplicity, we assume that the spin pattern may by locally represented by the Nèel state it is clear that the fast motion of a hole created in such a background mediated by the hopping term in the Hamiltonian creates defects (magnons) in the magnetic structure which raises the magnetic contribution to the energy. That rise tends to localize holes and thus it turns out that a convenient representation for quasiparticles in weakly doped AF is a SP state defined as a hole oscillating in a cloud of magnons created by its motion and trying to localize it. Those magnons form strings pinning holes to initial sites. Thus, the polaron wavefunction may be interpreted as a solution of a Schrödinger equation for a particle in a potential well with the center at a site where a hole has been initially created. Similar construction may be repeated for a pair of holes created at nearest neighbor sites. By definition, all processes which give rise to delocalization are omitted in the trial Hamiltonian that defines those potential wells. The Schrödinger equations which define a SP or a SPB incorporate processes related to the fast motion of holes with the rate $\sim t$ and count the diagonal part of the exchange energy. By applying the full Hamiltonian to the SP basis of states we derive an effective Hamiltonian, which also incorporates processes that have been neglected at an earlier stage of the calculation. The most obvious process which gives rise to coherent propagation of a single qusiparticles may be described in the following way. A pair of defects in the AF pattern of spins created by two consecutive hops of a hole which has been initially inserted at a given site into the perfect AF background, may be removed by applying the transversal part of the exchange term in the Hamiltonian. Since the final state represents a hole created in the ideal AF environment while the intermediate state corresponds to a string pinned to the initial site that process couples couples SPs localized at different sites. Lowest order coupling between different SBPs may be understood in a similar way. Let us consider a hole, a defect and a second hole which lie in a row on three nearest sites. Such a state may be obtained in two ways from a state that represents just two holes in the AF background. In the first case holes initially occupy the left pair of involved sites, while in the second the right pair. In both cases the hole in the middle site hops outwards the second hole. Since the final state represents a string states pinned to different pairs of sites, we notice that SBP states overlap. If the hole initially created at the outer site follows the hole which has made the first move, a state is obtained which represents a pair of bare holes shifted by one lattice spacing. Since the hop is mediated by the kinetic-energy term in the Hamiltonian, that process couples string states related to SPBs localized at different sites and gives rise to an off-diagonal term in the effective Hamiltonian. The annihilation of magnons by the transverse part of the exchange term may bring about a transformation of a SPB into a pair of SPs (and *vice versa*). It is clear that such an effect will be produced if two magnons are removed from a string that connects a pair of holes. Without dwelling much upon details we present now the form of the effective Hamiltonian expressed in terms of operators h_i and $h_i^\dagger$ annihilating and creating spin polarons.

$$
\begin{aligned}
\hat{H} - \mu\hat{N} = {} & (E_1 - \mu)\sum_i h_i^\dagger h_i + h \sum_{i,\delta,\delta';\, \delta'\neq-\delta} h_{i+\delta+\delta'}^\dagger h_i \\
& + (E_2/2 - E_1 + u_1)\sum_{i,\delta} h_i^\dagger h_{i+\delta}^\dagger h_{i+\delta} h_i \\
& + u_2 \sum_{i,\delta,\delta';\, \delta'\neq-\delta} h_i^\dagger h_{i+\delta+\delta'}^\dagger h_{i+\delta+\delta'} h_i + u_3 \sum_{i,\delta,\delta';\, \delta'\perp\delta} h_i^\dagger h_{i+\delta+\delta'}^\dagger h_{i+\delta+\delta'} h_i \\
& + u_4 \sum_{i,\delta,\delta',\delta'';\, \delta'\neq-\delta,\delta''\neq-\delta'} h_i^\dagger h_{i+\delta+\delta'+\delta''}^\dagger h_{i+\delta+\delta'+\delta''} h_i
\end{aligned}
$$

$$
\begin{aligned}
&+s_1 \sum_{i,\delta,\delta';\ \delta'\neq-\delta} h^\dagger_{i+\delta+\delta'} h^\dagger_{i+\delta} h_{i+\delta} h_i \\
&+s_2 \sum_{i,\delta,\delta',\delta'';\ \delta'\neq-\delta,\delta''\neq-\delta'} h^\dagger_{i+\delta+\delta'} h^\dagger_{i+\delta+\delta'+\delta''} h_{i+\delta} h_i \\
&+s_3 \sum_{i,\delta,\delta';\ \delta'\perp\delta} [(h^\dagger_i h^\dagger_{i+\delta+\delta'} h_{i+2\delta} h_i + H.c.) + h^\dagger_i h^\dagger_{i+\delta+\delta'} h_{i+\delta-\delta'} h_i] \\
&+s_4 \sum_{i,\delta,\delta',\delta'';\ \delta'\neq-\delta,\delta''\neq-\delta'} (h^\dagger_i h^\dagger_{i+\delta+\delta'+\delta''} h_{i+\delta} h_i + H.c.) \\
&+s_5 \sum_{i,\delta,\delta';\ \delta'\perp\delta} h^\dagger_i h^\dagger_{i+\delta'} h_{i+\delta} h_i \\
&+s_6 \sum_{i,\delta,\delta',\delta'';\ \delta'\neq\delta,\delta''\neq-\delta} (h^\dagger_{i+\delta+\delta''} h^\dagger_{i+\delta'} h_{i+\delta} h_i + H.c.) \\
&+s_7 \sum_{i,\delta,\delta';\ \delta'\perp\delta} h^\dagger_{i+\delta+\delta'} h^\dagger_{i+\delta'} h_{i+\delta} h_i
\end{aligned}
$$

δ denotes links to nearest neibhbor sites. E_1 and E_2 are eigenenergies of a SP and a SBP respectively. Other parameters are functions of J, t and amplitudes of string states in the solution of Schrödinger equations which define the SP and SBP.

We have analyzed appearance of superconductivity in the effective model by means of the mean field approach. The behavior of anomalous Green's functions in the region of low doping rougly agrees with results of the numerical calculation of Sorella and colloborators [1]. We observe that the SC order parameter vanishes in the limit of low hole doping, which may be attributed to emptying the spin polaron band and approaching the Mott insulator (MI) phase in the nominally half-filled system. Vanishing of the SC energy gap related to the coherent SC state does not necessarily mean that the underdoped AF should reveal features of an ordinary Fermi liquid-like normal state, because the system of freely propagating spin polarons becomes unstable against formation of bipolarons [3] which brings about opening of a pseudogap in the spectral function of a single quasiparticle.

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