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SPIN POLARONS IN TWO-DIMENSIONAL SYSTEMS

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The problem of motion of holes on a square lattice of antiferromagnetically ordered spins is considered. An overview of the theory of hole dynamics in the antiferromagnetic background is presented. Motion of a single hole is rather well understood both by numerical and analytical methods. For small but finite concentration of holes a treatment analogous to the standard polaron theory is discussed starting with an exact mapping of the $t-J$ Hamiltonian into holon and pseudospin variables.

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1. Introduction

In efforts to understand properties of high-T_c superconductors the problem of energy spectrum and correlated motions of electrons in CuO_2 planes evolved as one of the basic challenges. It is known from experiment that stoichiometric cuprates are spin-1/2 antiferromagnets with strong exchange interaction within CuO_2 planes [1, 2] and very weak interplane exchange coupling. Although the weak interplane exchange interaction is essential to stabilise long-range antiferromagnetic order at finite temperatures, normal state properties of superconducting cuprates are dominated by strong two-dimensional antiferromagnetic correlations resulting from large intraplanar exchange coupling [3, 4].

Band structure calculation (see e.g. [5]) combined with effects of many-body electron interactions treated in terms of multiband Hubbard Hamiltonian (see [6, 7] for reviews) lead to the conclusion that CuO_2 planes can be approximately described by an effective single narrow band Hubbard Hamiltonian (with, perhaps, hopping to second and third neighbours included [5]). The effective single band electron systems given by the Hubbard Hamiltonian $\mathcal{H} = -\sum_{i,j,\sigma} t c^+_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$ in the strong coupling regime $U \gg t$ can be approximately transformed [8] to the well-known $t-J$ model, restricted to the space with no double-occupied sites

$$\mathcal{H}_{t-J} = -\sum_{\langle i,j\rangle,\sigma} t X^+_{i\sigma} X_{j\sigma} + \frac{1}{2} J \sum_{\langle i,j\rangle} \left(s_i \cdot s_j - \frac{1}{4} n_i n_j \right), \tag{1}$$

where $X_{j\sigma} = c_{j\sigma}(1-n_{j\sigma})$, $n_{j\sigma} = X^+_{j\sigma}X_{j\sigma}$, $s^+_j = X^+_{j\uparrow}X_{j\downarrow}$, $s^z_i = \frac{1}{2}(n_{j\uparrow} - n_{j\downarrow})$, $n_j = \sum_\sigma n_{j\sigma}$, $J = 4t^2/U$. The formal equivalence of $\mathcal{H}_{t-J}$ with $\mathcal{H}$ in the limit $U \gg t$ was proven for the nearest neighbour hopping t with summation restricted to pairs $\langle i,j\rangle$ of nearest neighbours. Extension of (1) to second, etc. neighbours in fact implies neglecting some terms in the transformation leading to (1), [8]. In the half-filling case i.e. one electron per site $n_{i,-\sigma} = 1$ $\mathcal{H}_{t-J}$, (1), reduces to the spin-1/2 Heisenberg Hamiltonian having antiferromagnetic ground state. The situation close to half-filling, with a small concentration of excess electrons or holes was extensively studied in recent years and will be the topic of the present discussion.

A naive model of the CuO_2 planes would assume Cu^{2+} ions, each having one electron of uncompensated spin (or, rather, one hole in the otherwise occupied ionic d-shell) sitting at the sites of quadratic lattice, with O^{2-} ions between Cu^{2+} ions. However, $\mathcal{H}_{t-J}$ is an *effective* Hamiltonian approximating the more realistic 3-band minimal model (see e.g. [6]) in which the uncompensated spins belong to the Zhang–Rice (ZR) singlets [9]. The ZR singlets are bound states of d electrons from Cu and p electrons from O and are localised not exactly at the Cu sites. Still, the Hamiltonian (1) with a realistic choice of parameters J and t (along with, perhaps, t' and t'') captures essential physics of an excess carrier moving in antiferromagnetically ordered background of spin-1/2 electrons (holes). The case of nearest neighbour hopping t will be discussed mainly. The second- and third-neighbours hoppings t' and t'' will be included while comparing the theory with experiment, although t' and t'' contributions imply approximations of unchecked validity.

2. Motion of a hole in 2^d quantum antiferromagnet

An antiferromagnet on a quadratic lattice is composed of two equivalent interpenetrating sublattices, say A and B, so that each site from a given sublattice is surrounded by sites with opposite direction of the spin, apart from the ground state quantum fluctuations. A single hole can only move together with reversals of spins on its way. Reversal of a spin costs $2J$ in exchange energy so (if, for a moment, the quantum fluctuations, acting through the transverse spin components are neglected) the exchange energy cost would be proportional to the length of the path of the hole thus tending to trap it in the original site [10]. The energy spectrum of finite antiferromagnetic (AF) lattices with a single hole was extensively studied numerically, mainly by exact direct diagonalization [11, 12], see [13] for a review. To study the motion of a hole in the AF background under the constraint of no double-occupancy it was proposed ([14], see also [15]) to define hole operators h_i, obeying the Fermi statistic (but spinless) and hard core boson operators b_i: $c_{i\uparrow} = h^+_i$ but $c_{i\downarrow} = h^+_i S^+_i$ and $b^+_i = S^-_i$ on the $\uparrow$ sublattice and $b^+_i = S^+_i$ on the $\downarrow$ sublattice. The hopping part of $\mathcal{H}_{t-J}$, (1), can be now replaced [14] by

$$\mathcal{H}_t = t\sum_{\langle i,j\rangle} h^+_i h_j [b^+_j(1-b^+_i b_i) + (1-b^+_j b_j)b_i]. \tag{2}$$

Although (2) satisfies constraints on the motion of a hole [14], simplification of $\mathcal{H}_t$ into a tractable form $\mathcal{H}_t \cong t\sum_{\langle i,j\rangle} h^+_i h_j (b^+_j + b_i)$ brings the problem into a space

with redundant non-physical states. A formal remedy was proposed [15]. We shall come to this point in more rigorous way below.

Applying the standard linear spin wave (LSW) theory to map the spin operators $S_i^{\pm}$ into antiferromagnetic magnon operators ζ_q the transport Hamiltonian (2) was brought [14] into the form

$$\mathcal{H}_t = 4tN^{-1/2}\sum_{kq} P(\boldsymbol{k},\boldsymbol{q})h_k^+ h_{k-q}\zeta_q + \text{h.c.}, \tag{3}$$

where h_k is the Fourier transform of the holon operator h_i and $P(\boldsymbol{k},\boldsymbol{q})$ will be specified later on. The exchange term in (1) in the LSW-approximation has the usual form

$$\mathcal{H}_J = \sum_q \omega_q \zeta_q^+ \zeta_q, \tag{4}$$

apart from a constant.

The t–J model approximated by $\mathcal{H}_{t-J} = \mathcal{H}_t + \mathcal{H}_J$, (3) and (4), describes thus a peculiar motion of a hole driven only by its interaction with AF-magnons.

The problem of motion of the hole formally resembles the polaron problem [16] with AF-magnons playing now the role of phonons in (lattice) polarons. The important difference now is the absence of a direct kinetic energy of holes (in the model of only nearest-neighbour hopping), only magnon-assisted motion of holes is possible. The energy of a hole is calculated from the Green function [14, 15] defined by

$$G(\boldsymbol{k},\omega) = \left\langle 0|h_k \frac{1}{\omega - \mathcal{H}_{t-J}} h_k^+|0\right\rangle, \tag{5}$$

where $|0\rangle$ is the vacuum for holes and magnons, i.e. quantum antiferromagnetic ground state of the spin system with zero-point fluctuations. The energy of the state $|0\rangle$ is taken as zero. The Green function (5) was calculated in the self-consistent Born approximation (SCBA) [14, 15], $G(\boldsymbol{k},\omega) = 1/[\omega - \sum(\boldsymbol{k},\omega)]$ where the hole self-energy $\sum(\boldsymbol{k},\omega)$ is given by the equation

$$\sum(\boldsymbol{k},\omega) = (4t)^2 N^{-1}\sum_q [P(\boldsymbol{k},\boldsymbol{q})]^2 G(\boldsymbol{k}-\boldsymbol{q},\omega-\omega_q). \tag{6}$$

Self-consistent solutions of (6) were discussed qualitatively [14, 17] and obtained numerically [15, 18]. Results are best described by the spectral function $F(\boldsymbol{k},\omega) = -\frac{1}{\pi}\text{Im}G(\boldsymbol{k},\omega+\text{i}O)$. Numerical solutions of Eq. (6) in 2 dimensions were discussed in detail in Refs. [15, 18], general features of the solutions are qualitatively the same as of the earlier calculations for 1 dimension [14]. The spectral function $F(\boldsymbol{k},\omega)$ generally has a well-defined peak near the bottom of the spectrum, which corresponds to a quasiparticle, and a broad, incoherent part [14, 15, 18]. The quasiparticle consisting of a hole dressed in a cloud of virtual magnons is referred as a spin polaron by an obvious analogy with the well-known lattice polarons.

The magnon energy ω_q in (4) is proportional to J $(= 4t^2/U)$ whereas the magnon–hole interaction (3) is scaled by t. Relevant to experiment is the strong coupling case $J/t = 4t/U \ll 1$, there is no a priori proof that the self-consistent Born approximation (6) is accurate enough. Good quantitative agreement with results of numerical simulations, discussed below, is the justification of using SCBA.

In the weak coupling limit $t \ll J$ the perturbation calculations are expected to be correct. In this limit it is possible to solve (5) and (6) analytically [15] for the quasiparticle energy $\varepsilon_k = -\frac{(4t)^2}{N}\sum_q [P(k,q)]^2/\omega_q$. There are several fundamental questions pertaining to the results outlined above. First, one can ask why the SCBA works so well as can be judged from the good agreement with exact numerical computations for the cases with a single hole. The plausible answer is that the vertex corrections for the system described by Eqs. (3) and (4) are small [19]. The validity of the SCBA is further corroborated by a careful variational approach to a single-hole problem in the intermediate-coupling regime [20] (see also [21]). An interesting problem of the space structure of spin polarons was studied using the "exact", within SCBA, polaron wave function [22], see [23, 24]. From the SCBA wave function [22] it is possible to prove that the spin polaron spectral weight is non-vanishing in the thermodynamic limit, contrary to an earlier criticism. Thus, the motion of a single hole in AF background seems to be well understood, both by numerical and analytical methods*. For finite concentration of holes two kinds of problems arise. First, it was shown that non-uniform distributions of holes or the so-called stripe phases can be favourable energetically (see, e.g. [25]). Second, the constraints of no double-occupancy which are effectively lost in making approximations (LSW) to get Eq. (6) have to be more carefully treated for finite concentration of holes. This will be the centre of the discussion to follow.

3. Spin-charge separation and exact mapping of $\mathcal{H}_{t-J}$

The compelling physical arguments leading to Eq. (2) have to be augmented by an exact mapping of electron operators into spinless fermionic operators — holons, and (pseudo-) spin variables.

The idea of decoupling an electron operator into a holon, and a local spin (or pseudospin) was used quite extensively in studying the $t-J$ model. The central problem of the spin-charge separation is to properly take into account constraints on artificially extended Hilbert space. In the space of no double-occupied states, which has to be used for the $t-J$ model, the local Hilbert space for a given site i consists of three states: $|i\sigma\rangle$, an electron of $\sigma = \uparrow$ or $\downarrow$, and a hole at i, $|i0\rangle$. In the charge-separation model the local Hilbert space is a tensor product of holon and (pseudo-) spin space, $|\text{holon}\rangle_h \otimes |\text{spin}\rangle_S$ spanned over 2×2 local states, $|i0\uparrow\rangle$, $|i0\downarrow\rangle$, $|i1\uparrow\rangle$ and $|i1\downarrow\rangle$. The correspondence $|i0\rangle \to |i0\sigma\rangle$ is obvious but since there is no real spin at the site occupied by a holon, none of the states $|i1\uparrow\rangle$ or $|i1\downarrow\rangle$ has a direct physical meaning and one of them is redundant. The correspondence $|i0\rangle \to |i1\uparrow\rangle$ was assumed [26], discarding $|i1\downarrow\rangle$ as a non-physical state. Such procedure is unsatisfactory since it violates the time reversal symmetry of the original $t-J$ Hamiltonian. However, the transport term of the derived [26] $\mathcal{H}_{t-J}$ although not time-reversal symmetric in the LSW-approximation appeared equivalent to Eq. (3). Again, this approximation spoils the constraints by allowing a holon and spin deviation to appear at the same site. The problem with the

*It is interesting to note that anomalies in the extreme strong coupling regime $J \to 0$ or $U \to \infty$, as seen e.g. in Fig. 2 of Ref. [20], are compatible with the well-known Nagaoka theorem stating that a single hole in an otherwise half-filled Hubbard system in the limit $U \to \infty$ stabilises strongly ferromagnetic ground state.

LSW-approximation resembles closely the old problem of kinematical interactions of the spin-wave theory [27], perhaps also in the present system disregarding constraints does not influence significantly low energy states. A mapping of the $\mathcal{H}_{t-J}$ into holon-spin space conserving the time-reversal symmetry was derived by Wang and Rice [28]

$$\mathcal{H} = -t \sum_{\langle i,j \rangle} e_i e_j^+ \left(\frac{1}{2} + 2\boldsymbol{S}_i \cdot \boldsymbol{S}_j \right)$$

$$+(J/2) \sum_{\langle i,j \rangle} (1 - e_i^+ e_i) \left(\boldsymbol{S}_i \cdot \boldsymbol{S}_j - \frac{1}{4} \right) (1 - e_j^+ e_j). \tag{7}$$

Here we stick, for further convenience, to the original [28] notation where e_i, e_j^+ are holon operators and $\boldsymbol{S}_j$ are the local (or pseudo-) spin operators related to the true ones s_i by $s_i = (1-e_i^+ e_i)\boldsymbol{S}_i$. It is thus necessary to eliminate explicitly non-physical states for terms like $e_j^+ \boldsymbol{S}_j$ in (7). An alternative mapping of electron operators into holons and (pseudo-) spins was proposed [29]. Like in the Wang and Rice (WR) treatment [28] (in the space of no double-occupied states) the local Hilbert space of a site i complete with two spin states $|i\uparrow\rangle$, $|i\downarrow\rangle$ of an electron and the state $|i0\rangle$ of a hole at i is mapped into the $|\text{holon}\rangle \otimes |\text{spin}\rangle$ space by the correspondence [29]

$$|i\sigma\rangle \to |i0\rangle_h |i\sigma\rangle_S, \qquad |i0\rangle = |i1\rangle_h |iS\rangle_S, \tag{8}$$

where $|i0\rangle_h$ and $|i1\rangle_h$ are the holon states with occupations 0 and 1, respectively. The two local spin states are $|i\sigma\rangle_S$. At the site occupied by a hole, $|i1\rangle_h$, the local "fictitious" spin state $|iS\rangle_S$ is defined as the superposition [29] $|iS\rangle_S = c_1|i\uparrow\rangle_S + c_2|i\downarrow\rangle_S$ with arbitrary c_1, c_2 except for the normalization condition $|c_1|^2+|c_2|^2 = 1$. The local $|\text{holon}\rangle \otimes |\text{spin}\rangle$ space is now spanned on 4 states: $|i0\rangle_h|i\sigma\rangle_S, |i1\rangle_h|iS\rangle_S$, and $|i1\rangle_h|i\overline{S}\rangle_S$, where $|i\overline{S}\rangle_S$ is taken [29] as orthogonal to $|i\overline{S}\rangle_S$, i.e. $|i\overline{S}\rangle_S = c_1^*|i\downarrow\rangle - c_2^*|i\uparrow\rangle$. $|i\overline{S}\rangle_S$ is a non-physical state. The $t-J$ Hamiltonian (1) can be expressed in terms of the Hubbard operators $X_{i\sigma} = c_{i\sigma}(1 - n_{i,=\sigma})$, remembering that $n_{i\sigma} = X_{i,\sigma}^+ X_{i\sigma}$, $s_i^+ = X_{i\uparrow}^+ X_{i\downarrow}$ etc. In the initial local Hilbert space $\{|i\sigma\rangle, |i0\rangle\}$ $X_{i\sigma}$ can be represented as $X_{i\sigma} = |i0\rangle\langle i\sigma|$. In the local holon space $e_i^+|i0\rangle_h$, $e_i|i1\rangle_h = |i0\rangle_h$, $S_i^+|i\downarrow\rangle_S = |i\uparrow\rangle_S$, $S_i^-|i\uparrow\rangle_S = |i\downarrow\rangle_S$ so $e_i^+ = |i1\rangle_h\,{}_h\langle i0|$ etc. A simple algebra now can be used [29] to implement the correspondence (8) into a correspondence of the Hubbard operators, $X_{i\sigma} \to \widetilde{X}_{i\sigma}$ and then $\mathcal{H}_{t-J} \to \mathcal{H}$ into an equivalent form $\mathcal{H}$ in the $|\text{holon}\rangle\otimes|\text{spin}\rangle$ space. The transformed Hamiltonian $\mathcal{H}_{t-J}$ has to be time-reversal symmetric. This requirement imposes the condition [29] on the amplitudes: $|c_1| = |c_2|$. Thus $|c_1| = \frac{1}{\sqrt{2}}$, $c_2 = \frac{1}{\sqrt{2}}e^{i\varphi}$ with an arbitrary phase factor φ having no effect on physical quantities. In what follows $\varphi = 0$ is taken. The correspondence (8) thus leads to the relations $n_{i\uparrow} = (1 - e_i^+ e_i)S_i^+ S_i^-$, $n_{i\downarrow} = (1 - e_i^+ e_i)S_i^- S_i^+$, $s_i^\pm = (1 - e_i^+ e_i)S_i^\pm$, $s_i^z = (1 - e_i^+ e_i)S_i^z$, and $n_i = 1 - e_i^+ e_i$. Here $S_i^\pm$, S_i^z are the local spin-1/2 operators or rather pseudospin operators as they are real spin operators only if the site i is occupied by the electron, i.e. $1 - e_i^+ e_i = 1$ or there is no hole at i, $e_i^+ e_i = 0$. It is important to note [29] that the transformed Hubbard operators have no nonzero matrix elements for non-physical states $|i1\rangle_h|i\overline{S}\rangle_S$ since [29] $\widetilde{X}_{i\sigma}|i1\rangle_h|i\overline{S}\rangle_S = 0 = \widetilde{X}_{i\sigma}^+|i1\rangle_h|i\overline{S}\rangle_S$. Consequently, the

following transformed $t-J$ Hamiltonian acts in the (single-occupied) space of states having physical meaning [29]:

$$\mathcal{H} = -t\sum_{\langle i,j\rangle} e_i e_j^+ \frac{1}{2}(f_{ij}+g_{ij}) + \frac{1}{2}J\sum_{\langle ij\rangle}(1-e_i^+e_i)\left(\boldsymbol{S}_i\cdot\boldsymbol{S}_j - \frac{1}{4}\right)(1-e_j^+e_j), \quad (9)$$

where $f_{ij} = 2\boldsymbol{S}_i\cdot\boldsymbol{S}_j+\frac{1}{2}$, and $g_{ij} = S_i^+(\frac{1}{2}+S_j^z)+(\frac{1}{2}-S_i^z)S_j^+ + S_i^-(\frac{1}{2}-S_j^z)+(\frac{1}{2}+S_i^z)S_j^-$ and the components of $\boldsymbol{S}_i$ satisfy the usual commutation relations for spin 1/2. The only but important difference between Eqs. (7) and (9) is that instead of f_{ij} in (7) there is $\frac{1}{2}(f_{ij}+g_{ij})$ in (9). The contributions f_{ij} and g_{ij} in (9) have the same matrix elements if acting on physical states whereas they cancel each other if acting on non-physical states [29]. In the LSW-approximation the term $\sim \frac{1}{2}g_{ij}$ reproduces directly the one-magnon hopping term (3), however with reduced strength: $t \to \frac{1}{2}t$. Both forms, (7) and (9) are equivalent in the space of physical states [29].

4. Spin polarons in 2^d antiferromagnetic systems. Finite concentration

The Hamiltonian $\mathcal{H}$ of Eq. (9) will be now applied to a quadratic lattice of sites single-occupied by electrons except a number of holes with low concentration, $x = (1/N)\sum_i\langle e_i^+e_i\rangle \ll 1$ — a system modelling CuO_2 planes in cuprates. For $x = 0$ the system has antiferromagnetic ground state, the square lattice can be built up from two equivalent interpenetrating sublattices, say A and B such that a lattice site $j \in A$ of electron spin up at the ground state has as its nearest neighbours lattice sites $i \in B$ with spin down. To apply the spin-wave theory to an antiferromagnetic system it is a convenient procedure to apply to the exchange Hamiltonian an unitary transformation T reversing spin directions on one sublattice, say B thus changing the antiferromagnetic Néel state into a ferromagnetic one with a new Hamiltonian $T\mathcal{H}T^{-1}$. In applying such standard transformation one has to remember that $\boldsymbol{S}_i$ are not real spins but pseudospins and they have meaning only if a given site i is not occupied by a hole. This aspect seems to be overlooked in widely using the transformation T which changes $S_i^\pm \to S_i^\mp$, $S_i^z \to -S$ for i belonging to the sublattice, say B, and leaving $S_j^\pm$, S_j^z unchanged if $j \in A$, irrespective of the fact if there is/or not a hole at a given site. The correct transformation T is defined [26] as a product of local transformations T_l for all sites, $T = \Pi_l T_l$ where

$$T_l = \begin{cases} 1 & \text{if} \quad l = j \in A \\ (1-e_i^+e_i)(S_i^+ + S_i^-) + e_i^+e_i & \text{if} \quad l = i \in B. \end{cases} \quad (10)$$

For $j \in A$, $i \in B$ we have $Te_ie_j^+f_{ij}T^{-1} = e_ie_j^+\tilde{g}_{ij}$ and $Te_ie_j^+g_{ij}T^{-1} = \tilde{f}_{ij}$, where $\tilde{f}_{ij}$ and $\tilde{g}_{ij}$ are obtained by the substitution ($S_i^\pm \to S_i^\mp$, $S_i^z \to -S_i^z$) from f_{ij} and g_{ij}, respectively. This property corroborates the equivalence of (7) and (9), not so obvious from the first sight as in the lowest order LSW approximation g_{ij} leads to one-magnon scatterings of holes whereas f_{ij} implies two-magnon ones. It is thus convenient to take the transport part in the form implied by Eq. (7), i.e. $-t\sum_{\langle i,j\rangle} e_ie_j^+f_{ij}$ which after the transformation T is $\mathcal{H}_t = -t\sum_{\langle i,j\rangle} e_ie_j^+\tilde{g}_{ij}$.

The transformed exchange part $\mathcal{H}_J$ from (7) can be rewritten so as to clarify its physical contents

$$\mathcal{H}_J = \frac{J}{2}\sum_{\langle i,j\rangle}\left(S_{ij} - \frac{1}{4}\right) - J\sum_{\langle i,j\rangle} e_i^+ e_i(1 - e_j^+ e_j)S_{ij}$$
$$+\frac{J}{4}\sum_{\langle i,j\rangle} e_i^+ e_i(1 - e_i^+ e_i) - \frac{J}{2}\sum_{\langle i,j\rangle} e_i^+ e_i\left(S_{ij} - \frac{1}{4}\right) e_j^+ e_j, \tag{11}$$

$S_{ij} = \frac{1}{2}(S_i^+ S_j^+ + S_i^- S_j^-) - S_i^z S_j^z$, for brevity. The first term of the right side of (11) is the usual Heisenberg type exchange Hamiltonian $\mathcal{H}_{\rm ex}^0$ for the half-filling situation, the third term is independent on magnetic state of the system and determines corrections to the holon energy due to presence of other holons. The last term can be neglected for small concentration of holes since the probability of finding two holons on nearest neighbouring sites is very small. The second term describing deformations of the antiferromagnetic background by the hole is nontrivial as the (pseudo-) spin $\boldsymbol{S}_i$ is not defined at the site occupied by a hole. This term will be approximated by averaging the contributions occupied by holes over the local spin states $|iS\rangle_S$. Thus $\mathcal{H}_J$, Eq. (11), is reduced to [30]

$$\mathcal{H}_J = \mathcal{H}_{\rm ex}^0 + \frac{J}{4}\sum_{\langle i,j\rangle} e_i^+ e_i(1 - e_j^+ e_j) - \frac{J}{4}\sum_{\langle i,j\rangle} e_i^+ e_i(S_j^- + S_j^+)(1 - e_j^+ e_j). \tag{12}$$

In the last two terms of (12), for small concentration of holes $x = \langle e_j^+ e_j\rangle$, $J(1 - e_j^+ e_j)$ can be approximately replaced by $\overline{J} = J(1 - x)$.

In linear spin wave theory the spin operators are expressed in terms of bosons: $S_l^- \cong a_l$, $S_l^+ \cong a_l^+$, $S_l^z = a_l^+ a_l - \frac{1}{2}$. The unperturbed exchange part $\mathcal{H}_{\rm ex}^0 = \frac{J}{2}\sum_{\langle i,j\rangle}(-S_i^z \cdot S_j^z + \frac{1}{2}S_i^+ S_j^+ + \frac{1}{2}S_i^- S_j^- - \frac{1}{4})$ can be diagonalized by the standard Fourier transformation $a_i = N^{-1/2}\sum_q e^{i\boldsymbol{q}\cdot\boldsymbol{R}_i}\alpha_q$ followed by the Bogolyubov canonical transformation $\alpha_q = u_q\zeta_q + v_q\zeta_{-q}^+$ where $u_q = \cosh\Theta_q$, $v_q = \sinh\Theta_q$, $\tanh 2\Theta_q = -\gamma_q$ and $\gamma_q = (1/4)\sum_\delta e^{i\boldsymbol{q}\cdot\boldsymbol{\delta}} = \frac{1}{2}(\cos q_x + \cos q_y)$, $\boldsymbol{\delta}$ are vectors to nearest neighbours in the quadratic lattice. $\mathcal{H}_J$ (or, strictly, $T\mathcal{H}_J T^{-1}$) of Eq. (12) takes now the form

$$\mathcal{H}_J = \sum_q \omega_q\left(\zeta_q^+\zeta_q + \frac{1}{2}\right) + \overline{J}\sum_i e_i^+ e_i + \sum_q (F_q\zeta_q + F_q^+\zeta_q^+), \tag{13}$$

where $\omega_q = 2J\sqrt{1 - \gamma_q^2}$ is the (AF) magnon energy and $F_q = -N^{-1/2}\overline{J}\gamma_q \times (u_q + v_q)\rho_q$ with $\rho_q = \sum_i e_i^+ e_i e^{i\boldsymbol{q}\cdot\boldsymbol{R}_i}$. The linear term in magnon operators in Eq. (13) corresponds to the coupling of magnons to the holons density fluctuations. $\mathcal{H}_J$ is analogous to the Hamiltonian of a lattice polaron and similar approach can be used to eliminate the linear terms. The unitary transformation [31]

$$U = \exp\sum_q (F_q^+\zeta_q^+ - F_q\zeta_q)/\omega_q, \tag{14}$$

which acts as a simple shift transformation on magnon operators $U\zeta_q U^+ = \zeta_q - (F_q/\omega_q)$, applied to Eq. (13) leads to $\tilde{\mathcal{H}}_J = U\mathcal{H}_J U^{-1}$,

$$\tilde{\mathcal{H}}_J = \sum_q \omega_q\left(\zeta_q^+\zeta_q + \frac{1}{2}\right) + \sum_i e_i^+ e_i\overline{J}\left[1 - N^{-1}\sum_q \frac{\overline{J}\gamma_q^2}{\omega_q}(u_q^2 + v_q^2)\right]. \tag{15}$$

The transport Hamiltonian $\mathcal{H}_t$ in LSW approximation has the form

$$\mathcal{H}_t = -t \sum_{\langle i,j \rangle} e_i e_j^+ (a_i^+ + a_j). \tag{16}$$

The polaron transformation (14) strongly modifies $\mathcal{H}_t$ since

$$U e_i e_j^+ U^+ = e_i e_j^+ \Phi_{ij}, \qquad \Phi_{ij} = \exp N^{-1/2} \sum_q A_{ij}^q (\zeta_q - \zeta_{-q}^+), \tag{17}$$

where $A_{ij}^q = -\overline{J}(\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{R}_i} - \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{R}_j})\gamma_q(u_q + v_q)/\omega_q$. The band-narrowing factor Φ_{ij} involves multimagnon processes reminiscent to the multiphonon processes in the theory of lattice polarons. An approximate estimate of the effect of band narrowing is given by the average $\langle \Phi_{ij} \rangle$ over magnon states [30]. For nearest neighbours, $\boldsymbol{R}_i - \boldsymbol{R}_j = \boldsymbol{\delta}$:

$$\langle \Phi_\delta \rangle = \exp \left[-\frac{(1-x)^2}{4} N^{-1} \sum_q \gamma_q^2 (1-\gamma_q)^2 (1-\gamma_q^2)^{-3/2} \right]. \tag{18}$$

For small concentration of holes x the factor $\langle \Phi_\delta \rangle$ is significantly smaller from 1, cf. [30]. However, averaging of Φ_{ij} over magnon states implies mixing one-magnon effects with the higher order ones so it cannot be used for a systematic study. Instead a procedure was proposed [30] to pick-up one-magnon terms from $\widetilde{\mathcal{H}}_t$ and to approximate the remaining terms by their averages over magnon states, i.e. from (16)

$$\widetilde{\mathcal{H}}_t = U \mathcal{H}_t U^+ \cong -t \sum_{\langle i,j \rangle} e_i e_j^+ U (a_i^+ + a_j) U^+$$

$$-t \sum_{\langle i,j \rangle} e_i e_j^+ {}_m\langle 0 | (\Phi_{ij} - 1) U (a_i^+ + a_j) U^+ | 0 \rangle_m,$$

where $|0\rangle_m$ is the quantum AF ground state. The first term in $\widetilde{\mathcal{H}}_t$, after the usual Fourier transformation, with $e_i = N^{-1/2} \sum_k \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}_i} h_k$ and the Bogolyubov transformation, reproduces the known expression (3) and the second gives a small, concentration dependent, direct kinetic energy (see [30] for details, in slightly different notation)

$$\widetilde{\mathcal{H}}_t = \sum_k E_k^{(0)} h_k^+ h_k + 4t N^{-1/2} \sum_{kq} P(\boldsymbol{k}, \boldsymbol{q}) (h_k^+ h_{k-q} \zeta_q + \text{h.c.}), \tag{19}$$

where $P(\boldsymbol{k}, \boldsymbol{q}) = \gamma_{k-q} u_q + \gamma_k v_q$, and $E_k^{(0)} = 4t \mathcal{W}^{AB}(x) \gamma_k$. Roughly $\mathcal{W}^{AB}(x) \cong -0.5x$ [30], so $\mathcal{W}^{AB}(x)$ is small for the relevant range of x. The total free kinetic energy of holons E_k includes also dispersionless contribution listed as the second term in $\widetilde{\mathcal{H}}_J$ of Eq. (15) $E_k = \overline{J} \left[1 - N^{-1} \sum_q \frac{\overline{J}\gamma_q^2}{\omega_q} (u_q^2 + v_q^2) \right] + E_k^{(0)}$.

5. Conclusions

Two points are important in the present discussion. First, the arguments of Sec. 3 support the view, anticipated in the existing literature [14, 15] although not really proved that neglect of the constraints to the physical states as implied

by the LSW approximation still leads to correct, at least qualitatively, quasiparticle spectra. In particular, it was shown [32] that the quasiparticle dispersion relation (normalized to the quasiparticle band width) calculated in SCBA from (9) with $\frac{1}{2}(f_{ij} + g_{ij})$ with both 1- and 2-magnon processes taken into account or with $\frac{1}{2}(f_{ij} + g_{ij})$ replaced by g_{ij} and only 1-magnon processes considered, is the same within the computational error. Second, the polarons effects discussed in the previous section for finite x cannot be ignored. It is still an open question if it is a better approximation to use a reduced $t_{\rm ef} = t\langle\Phi_\delta\rangle$ in the transport term $\widetilde{\mathcal{H}}_t$ or adhere to the procedure of extracting only 1-magnon processes and throw the rest into an effective "free" kinetic energy of holons. Third, the model (1) with nearest-neighbour hopping only is not satisfactory. Band structure calculations [5] indicate that the CuO_2 planes can be modelled by a single band but with hoppings to next and next-next-nearest neighbours, t' and t'' included. Extensions to t' seem insufficient [33, 30]. Comparison of calculations of the holon dispersion with experimental data [34] is improved if t' and t'' is taken into account [35].

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