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DYNAMICS OF CARRIONS
IN THE SPIN-FERMION MODEL

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1 Introduction

A vast amount of theoretical searches for the relevant mechanism of high temperature superconductivity (HTSC) deals with the strongly correlated electron models [1] - [6]. Much attention has been devoted to the formulation of successful theory of the electrons (or holes) propagation in the CuO_2 planes in copper oxides. In particular, much efforts have been done to describe self-consistently the hole propagation in the doped 2D quantum antiferromagnet [7] - [30]. The understanding of the true nature of the electronic states in HTSC are one of the central topics of the current experimental and theoretical efforts in the field [2]. The plenty of experimental and theoretical results shows that the charge and spin fluctuations induced in the carrier hopping lead to the drastic renormalization of the single-particle electronic states due to the strong correlation. It makes the problem of constructing of the correct ground state wave functions and description the real many-body dynamics of the relevant correlated models of HTSC quite difficult [1] - [31]. The right picture of dynamical properties is very important issue, because of the most significant experimental data of HTSC have a dynamical nature, i.e. depends on frequency, [4]. The dramatic change of the electronic structure caused by the carrier doping is found in one-particle spectral density (e.g. [32]).

Theoretical description of strongly correlated fermions on two-dimensional lattices and the hole propagation in the antiferromagnetic background still remains controversial [30]. Furthermore, validity of different variants of perturbation expansions are not quite clear. The first attempts [7] - [21] to describe the hole propagation have shown clearly that the results depends strongly on the type of the model (2D Hubbard, t-J model, d-p model, etc), the choice of the background (RVB, Neel, triangular, etc) and the method of calculation. The role of quantum spin fluctuations was found to be quite crucial for the hole propagation [24].

The essence of the problem is in the inherent interaction (and coexistence) between charge and spin degrees of freedom which are coupled in a self-consistent way. The propagating hole perturbs the antiferromagnetic background and move then together with the distorted underlying region. In the "prophetic" language [33] of the gauge theory of holes in High-Tc superconductors it was called as a kind of quasiparticle "carrion", which is composed of the hole(electron) and the "cloud" of SU(2) Yang-Mills field around the hole. The perturbed gauge fields will be then spontaneously broken through Higgs-like mechanism to describe the situation when antiferromagnet symmetry is broken around the hole. There were many attempts [1] - [6] to realise this program. The significance of these attempts is, by no means, very important. However, a definite proof of the fully adequate mechanism for the coherent propagation of the hole is still lacking. The study of the hole quasiparticle propagation in the doped phase is still a quite open subject and is not well understood. In the present paper we will analyse the physics of the doped systems and the true nature of carriers in the 2D antiferromagnetic background from the many-body theory point of view. The dynamics of the charge degrees of freedom for the CuO_2 planes in copper oxides will be described in the framework of the spin-fermion (Kondo-Heisenberg) model [46] and compared with dynamics of other models. We shall use for this aim the Irreducible Green's Functions Method [34] - [36].

2 Irreducible Green's Functions Method

A number of perturbation approaches have been used to describe the spin and carrier dynamics of HTSC. In the present paper we use novel nonperturbative method to attack the same problem. This method of Irreducible Green Functions(IGF) [34] - [36],[43] rely on a unified self-consistent calculation of one-particle fermion and spin Green Functions(GF) including damping effects and finite lifetimes and gives the correct results both for the weak and strong coupling. The approach we suggest is founded on the number of studies and has proved to be valuable for the s-f model [37], [38], Heisenberg antiferromagnet [39], Anderson model [40], [41] and Hubbard model [42], [35]. In this paper it will be attempted to justify the use of IGF method for the description of the hole propagation in a quantum antiferromagnet. Our approach is in many respect complimentary and incorporate the logic of development of the many-body technique [36]. The study of the quasiparticle excitations in solids has been related deeply with the Green's Functions method [44] and has been one of the most fascinated subject for many years. We have developed the helpful reformulation [34] of the two-time thermodynamic GFs method which is especially adjusted for the correlated fermion systems on a lattice [43].

To clarify the foregoing, let us consider the retarded GF of the form

$$G^r(t-t') = \langle\langle A(t), B(t') \rangle\rangle = -i\theta(t-t') \langle [A(t)B(t')]_{\eta} \rangle; \eta = \pm 1. \quad (1)$$

The essence of the IGF method is as follows [34]. It is based on the notion of **IRREDUCIBLE** parts of GFs (or the irreducible parts of the operators, out of which the GF is constructed) in terms of which it is possible, without recursion to a truncation of the hierarchy of equations for the GFs, to write down the exact Dyson equation and to obtain an exact analytical representation for the self-energy operator. Let us consider the sketch of the method in a symbolic form. To calculate the GF (1) let us write down the equation of motion for it:

$$\omega G(\omega) = \langle [A, A^+]_{\eta} \rangle + \langle\langle [A, H]_- | A^+ \rangle\rangle_{\omega} \quad (2)$$

By definition we introduce the irreducible part ir of the GF

$$(\textit{ir} \langle\langle [A, H]_- | A^+ \rangle\rangle) = \langle\langle [A, H]_- - zA | A^+ \rangle\rangle \quad (3)$$

The unknown coefficient z is defined by special constraint, which is in core of the whole method

$$\langle [[A, H]_{-}^{\textit{ir}}, A^+]_{\eta} \rangle = 0 \quad (4)$$

From the condition (4) one can find:

$$z = \frac{\langle [[A, H]_{-}, A^+]_{\eta} \rangle}{\langle [A, A^+]_{\eta} \rangle} \quad (5)$$

Therefore, irreducible GF (3) is defined so that it cannot be reduced to the lower-order ones by any kind of decoupling. This procedure extract all relevant (for the problem under consideration) mean field contributions and put them into the generalized mean field GF, which is defined as [34]

$$G^0(\omega) = \frac{\langle [A, A^+]_{\eta} \rangle}{(\omega - z)}. \quad (6)$$

It is worthy to note that Generalized Mean Fields can have, in principle, a complicated structure for the system with strong interaction and complicated many-branch spectrum and are not reduced to the functional of the mean densities of the particles or quasiparticles. To calculate the IGF in (2), we have to write down the equation of motion after differentiation with respect to the second time variable t' . The constraint (4) remove the inhomogeneous term from this equation. If one introduces an irreducible part for the right-hand side operator, then the equation of motion (2) can be exactly (or identically) rewritten in the form of the Dyson equation

$$G = G^0 + G^0 M G \quad (7)$$

which has well known formal solution of the form

$$M = (G^0)^{-1} - G^{-1} \quad (8)$$

The full problem cannot be handled and one makes the approximations. Note that in contrast to the standard equation-of-motion approach, the decoupling is introduced in the self-energy operator only. The general philosophy of the IGF method lies in separation and identification of elastic scattering effects and inelastic ones. This last point is quite often underestimated. However, as far as the right definition of quasiparticle damping (i.e. true quasiparticles) is concerned, the separation of elastic and inelastic scattering processes is believed to be crucially important for the many-body systems with complicated many-branch spectrum and strong interaction. It was emphasized especially recently [45], that the anomalous damping of electrons (or holes) distinguishes cuprate superconductors from ordinary metals. It is worth mentioning that, in general, the mean-field renormalizations can exhibit a quite nontrivial structure. To obtain this structure correctly, one must construct the full GF from the complete algebra of relevant operators and develop a special projection procedure for higher-order GF's in accordance with a given algebra.

3 Hubbard model and t-J model

The model Hamiltonian which is usually referred as to Hubbard Hamiltonian is given by

$$H = \sum_{ij\sigma} t_{ij} a_{i\sigma}^\dagger a_{j\sigma} + \frac{U}{2} \sum_{i\sigma} n_{i\sigma} n_{i-\sigma} \quad (9)$$

For the strong coupling limit, when Coulomb integral $U \gg W$, where W is the effective bandwidth, the Hubbard Hamiltonian is reduced in the low-energy sector to t-J model Hamiltonian of the form

$$H = \sum_{ij\sigma} (t_{ij}(1 - n_{i-\sigma}) a_{i\sigma}^\dagger a_{j\sigma} (1 - n_{j-\sigma}) + H.C.) + J \sum_{ij} S_i S_j \quad (10)$$

This Hamiltonian play an important role in the theory of HTSC. The more refined and detailed derivations does not change the opinion that as regards to essential physics of HTSC this model is still instructive and workable. Let us consider the carrier motion.

The hopping at half-filling is impossible and this model describe the planar Heisenberg antiferromagnet. The most interesting problem is the behaviour of this system when the doped holes are added. In the $t - J$ model ($U \rightarrow \infty$) doped holes can move only in the projected space, without producing doubly occupied configurations ($\langle n_{\uparrow} \rangle + \langle n_{\downarrow} \rangle \leq 1$). There is then a strong competition between the kinetic energy of the doped carriers and the magnetic order present in the system. According to Ref. [19], it is possible to rewrite first term in (10) in the following form

$$H_t = t \sum_{\langle ij \rangle} (a_{i\uparrow}^{\dagger} S_i^{-} S_j^{+} a_{j\uparrow} + a_{i\downarrow}^{\dagger} S_i^{+} S_j^{-} a_{j\downarrow} + h.c.) \quad (11)$$

This form show clearly the nature hole-spin correlated motion over antiferromagnetic background. To describe in a self-consistent way a correlated motion of a carrier one need to consider the following complicated matrix Green's Function(c.f. [37], [38],[35]):

$$G(i, j) = \begin{pmatrix} \langle\langle a_{i\uparrow} | a_{i\uparrow}^{\dagger} \rangle\rangle & \langle\langle a_{i\uparrow} | a_{j\uparrow}^{\dagger} \rangle\rangle & \langle\langle a_{i\uparrow} | S_j^{+} \rangle\rangle & \langle\langle a_{i\uparrow} | S_j^{-} \rangle\rangle \\ \langle\langle a_{i\downarrow} | a_{i\downarrow}^{\dagger} \rangle\rangle & \langle\langle a_{i\downarrow} | a_{j\downarrow}^{\dagger} \rangle\rangle & \langle\langle a_{i\downarrow} | S_j^{+} \rangle\rangle & \langle\langle a_{i\downarrow} | S_j^{-} \rangle\rangle \\ \langle\langle S_i^{-} | a_{j\uparrow}^{\dagger} \rangle\rangle & \langle\langle S_i^{-} | a_{j\downarrow}^{\dagger} \rangle\rangle & \langle\langle S_i^{-} | S_j^{+} \rangle\rangle & \langle\langle S_i^{-} | S_j^{-} \rangle\rangle \\ \langle\langle S_i^{+} | a_{j\uparrow}^{\dagger} \rangle\rangle & \langle\langle S_i^{+} | a_{j\downarrow}^{\dagger} \rangle\rangle & \langle\langle S_i^{+} | S_j^{+} \rangle\rangle & \langle\langle S_i^{+} | S_j^{-} \rangle\rangle \end{pmatrix} \quad (12)$$

It may be shown after most straightforward but tedious manipulations by using IGF method that the equation of motion (2) for the GF (12) can be rewritten as a Dyson equation (7) for two-time thermodynamic retarded GF:

$$G(i, j; \omega) = G_0(i, j; \omega) + \sum_{mn} G_0(i, m; \omega) M(m, n; \omega) G(n, j; \omega) \quad (13)$$

The algebraic structure of the full GF in (13) which follows from (8) is rather complicated. For clarity, we illustrate some features by means of simplified problem.

4 Hole Spectrum of $t - J$ model

In paper [10] the idea to write down the special ansatz for fermionic operator as a composite operator of dressed hole operator and spin operator has been proposed for the case $J \gg t$. They introduced hole operator h_i corresponding to fermion operator $a_{i\sigma}^{\dagger}$ on the spin-up sublattice using the ansatz $a_{i\uparrow}^{\dagger} = h_i S_i^{-}$ and similarly for spin-down sublattice. Then the Hamiltonian (11) obtain the form

$$H_t = t \sum_{ij} I_{ij} h_j^{\dagger} h_i (b_i^{\dagger} + b_j) \quad (14)$$

Here b_i and b_j^{\dagger} are the boson operators, which results from the Holstein-Primakoff transformation of spins into bosons. Equation (14) is not convenient form because of its non-diagonal structure. Caution should be exercised because the new vacuum is a distorted Neel vacuum.

The equation of motion (2) and (3) for the hole GF can be written in the following form

$$\omega \langle\langle h_j | h_k^+ \rangle\rangle - t \sum_n I_{jn} \langle B_{nj} \rangle \langle\langle h_n | h_k^+ \rangle\rangle = \delta_{jk} + t \sum_n I_{jn} \langle\langle h_n B_{nj} | h_k^+ \rangle\rangle \quad (15)$$

Here $B_{nj} = (b_n^+ + b_j)$. The "mean-field" GF (6) is defined by

$$\sum_i (\omega \delta_{ij} - t I_{ij} \langle B_{ji} \rangle) G_0(i, k; \omega) = \delta_{jk} \quad (16)$$

Note, that "spin distortion" $\langle B_{mn} \rangle$ does not depend on $(R_m - R_n)$. According to eqs. (1) - (7), the Dyson equation (13) becomes

$$G(g, k) = G_0(g, k) + \sum_{j'l} G_0(g, j) M(j, l) G(l, k) \quad (17)$$

where self-energy operator is given by

$$M(j, l) = t^2 \sum_{mn} I_{jn} \langle\langle h_n B_{nj} | h_m^+ B_{km} \rangle\rangle I_{ml} \quad (18)$$

The standard IGF-method's prescriptions for the approximate calculation of the self-energy (c.f.[35], [37], [38]) can be written in the form

$$M(j, l; \omega) = t^2 \sum_{mn} I_{jn} I_{ml} \int_{-\infty}^{+\infty} d\omega_1 d\omega_2 \frac{1 + N(\omega_1) - n(\omega_2)}{\omega - \omega_1 - \omega_2} \quad (19)$$

$$\left(\frac{1}{\pi} \text{Im} \langle\langle B_{nj} | B_{lm} \rangle\rangle_{\omega_1} \right) \left(\frac{1}{\pi} \text{Im} G(l, m; \omega_2) \right)$$

In the present context, the three main weaknesses of the model (14) are the following. (i) The above presented formalism is relevant for quasi-static hole; (ii) The mass operator (19) is proportional to t^2 ; (iii) The standard iterative self-consistent procedure of IGF approach for the calculation of mass operator encounter the need of choosing as a first iteration "trial" solution the non-diagonal initial spectral function $\text{Im}G_0$. We shall see below that these drawbacks does not exist for the spin-fermion model.

The initial hole GF in paper [13] was defined as

$$G_0(j, k; \omega) = \frac{\delta_{jk}}{\omega + i\epsilon} \quad (20)$$

which corresponds to static hole, without dispersion. In contrast, the approximation for the magnon GF yield the momentum distribution of a free magnon gas. After integration in (19), the mass operator is given by an expression quite similar to the one encountered in papers [13], where the Bogolubov-de Gennes equations has been derived. These equations for the inhomogeneous superconducting samples plays an important role as it was argued in Ref.[7] in the context of high Tc superconductivity. It can be checked that the present set of equations (17) - (19) gives the finite temperature generalisation of the results[10],

[13]. As we just mentioned, one of its main merits is that it enables one to see clearly the "composite" nature of the hole states in an antiferromagnetic background, but, unfortunately, in the quasi-static limit. As a consequence, the formulation of the model, which tends to "reproduce" this composite nature of the carriers from the beginning, appears naturally if one wants to keep track of the relevant hole quasiparticle dynamics in copper oxides. This does not necessarily exclude the possibility of complementary studying of the both $t - J$ and spin-fermion models.

5 Spin-Fermion Model

As far as the CuO_2 -planes in the copper oxides are concerned, it was argued [46] that a suitable workable model with which one can discuss the dynamical properties of charge and spin subsystems is the spin-fermion (or Kondo-Heisenberg) model [47]. This model allows for motion of doped holes and results from d-p model Hamiltonian [2]. We consider the interacting hole-spin model for a copper-oxide planar system described by the Hamiltonian

$$H = H_t + H_K + H_J \quad (21)$$

where H_t is the doped hole Hamiltonian

$$H_t = - \sum_{\langle ij \rangle \sigma} (t a_{i\sigma}^\dagger a_{j\sigma} + H.C.) = \sum_{k\sigma} \epsilon(k) a_{k\sigma}^\dagger a_{k\sigma} \quad (22)$$

where $a_{i\sigma}^\dagger$ and $a_{i\sigma}$ are the creation and annihilation second quantized fermion operators, respectively for itinerant carriers with energy spectrum

$$\epsilon(q) = -4t \cos(1/2q_x) \cos(1/2q_y) = t\gamma_1(q). \quad (23)$$

The term H_J in (1) denotes Heisenberg superexchange Hamiltonian

$$H_J = \sum_{\langle mn \rangle} J \vec{S}_m \vec{S}_n = \frac{1}{2N} \sum_q J(q) \vec{S}_q \vec{S}_{-q} \quad (24)$$

Here \vec{S}_n is the operator for a spin at copper site \vec{r}_n and J is the u.n. superexchange interaction

$$J(q) = 2J[\cos(q_x) + \cos(q_y)] = J\gamma_2(q) \quad (25)$$

Finally, the hole-spin (Kondo type) interaction H_K may be written as (for one doped hole)

$$H_K = \sum_i K \vec{\sigma}_i \vec{S}_i = N^{-1/2} \sum_{kq} \sum_{\sigma} K(q) [S_{-q}^{-\sigma} a_{k\sigma}^\dagger a_{k+q-\sigma} + z_{\sigma} S_{-q}^z a_{k\sigma}^\dagger a_{k+q\sigma}] \quad (26)$$

This part of the Hamiltonian was written as the sum of a dynamic(or spin-flip) part and a static one. Here K is hole-spin interaction energy

$$K(q) = K[\cos(1/2q_x) + \cos(1/2q_y)] = K\gamma_3(q) \quad (27)$$

and sign factor z_σ is given by

$$z_\sigma = (+\text{or}-) \quad \text{for} \quad \sigma = (\uparrow \text{ or } \downarrow)$$

We start in this paper with the one doped hole model (21), which is considered to have captured the essential physics of the multi-band strongly correlated Hubbard model in the most interesting parameters regime $t > J, |K|$. We apply the IGF method to spin-fermion model (21). It will be shown that we are able to give a much more detailed and self-consistent description of the fermion and spin excitation spectra than in papers [47] - [53], including the damping effects and finite lifetimes.

6 Hole Dynamics in the Spin-Fermion Model

The two-time thermodynamic Green Functions to be studied here are given by

$$G(k\sigma, t - t') = \langle\langle a_{k\sigma}(t), a_{k\sigma}^+(t') \rangle\rangle = -i\theta(t - t') \langle [a_{k\sigma}(t), a_{k\sigma}^+(t')]_+ \rangle \quad (28)$$

$$\chi^{+-}(mn, t - t') = \langle\langle S_m^+(t), S_n^-(t') \rangle\rangle = -i\theta(t - t') \langle [S_m^+(t), S_n^-(t')]_- \rangle \quad (29)$$

In order to evaluate the GFs (28) and (29) we need use the suitable information about a ground state of the system. For the 2D spin 1/2 quantum antiferromagnet in a square lattice the calculation of the exact ground state is a very difficult problem [2] - [6]. In this paper we assume the two-sublattice Neel ground state. According to Neel model, the spin Hamiltonian (24) may be expressed as [34],[39]

$$H_J = \sum_{\langle mn \rangle} \sum_{\alpha, \beta} J^{\alpha\beta} \vec{S}_{m\alpha} \vec{S}_{n\beta} \quad (30)$$

Here $(\alpha, \beta) = (a, b)$ are the sublattice indices.

To calculate the electronic states induced by hole-doping in the spin-fermion model approach we need to calculate the energies of a hole introduced in the Neel antiferromagnet. To be consistent with (30) and (12) we define the single-particle fermion GF as

$$G(k\sigma, \omega) = \begin{pmatrix} \langle\langle a_a(k\sigma) | a_a^+(k\sigma) \rangle\rangle & \langle\langle a_a(k\sigma) | a_b^+(k\sigma) \rangle\rangle \\ \langle\langle a_b(k\sigma) | a_a^+(k\sigma) \rangle\rangle & \langle\langle a_b(k\sigma) | a_b^+(k\sigma) \rangle\rangle \end{pmatrix} \quad (31)$$

Note, that the same fermion operators $a_\alpha(i\sigma)$, annihilates a fermion with spin σ on the (α) -sublattice in the i -th unit cell has been used in paper [18]. The equation of motion for the Fourier transform of the elements of GF (11) are written as

$$\sum_{\gamma} (\omega \delta_{\alpha\gamma} - \epsilon^{\alpha\beta}(k)) \langle\langle a_\gamma(k\sigma) | a_\beta^+(k\sigma) \rangle\rangle = \delta_{\alpha\beta} \langle\langle A(k\sigma, \alpha) | a_\beta^+ \rangle\rangle \quad (32)$$

where

$$A(k\sigma, \alpha) = N^{-1/2} \sum_p K(p) (S_{-p\alpha}^{-\sigma} a_\alpha(k + p - \sigma) + z_\sigma S_{-p\alpha}^2 a_\alpha(k + p\sigma)) \quad (33)$$

We make use of the general Irreducible Green Function(IGF) approach [35],[36](see Section 2) to treat the the equation of motion (32). It may be shown that equation (32) can be rewritten as the Dyson equation (7) for two-time thermodynamic retarded GF

$$G(k\sigma, \omega) = G_0(k\sigma, \omega) + G_0(k\sigma, \omega)M(k\sigma, \omega)G(k\sigma, \omega) \quad (34)$$

Here $G_0(k\sigma, \omega) = \Omega^{-1}$ describes the behaviour of the electronic subsystem in the Generalized Mean-Field(GMF) approximation (for the detailed discussion of the GMF concept, see [35],[36]). The Ω matrix have the form

$$\Omega(k\sigma, \omega) = \begin{pmatrix} (\omega - \epsilon_a(k\sigma)) & -\epsilon^{ab}(k) \\ -\epsilon^{ba}(k) & (\omega - \epsilon_b(k\sigma)) \end{pmatrix} \quad (35)$$

where

$$\epsilon_\alpha(k\sigma) = \epsilon^{\alpha\alpha}(k) - z_\sigma N^{-1/2} \sum_p K(p) \langle S_{p\alpha}^z \rangle \delta_{p,0} = \epsilon^{\alpha\alpha}(k) - z_\sigma K S_z \quad (36)$$

$$S_z = N^{-1/2} \langle S_{0\alpha}^z \rangle$$

is the renormalized band energy of the holes.

The elements of the matrix GF $G_0(k\sigma, \omega)$ are found to be

$$G_0^{aa}(k\sigma, \omega) = \frac{u^2(k\sigma)}{\omega - \epsilon_+(k\sigma)} + \frac{v^2(k\sigma)}{\omega - \epsilon_-(k\sigma)} \quad (37)$$

$$G_0^{ab}(k\sigma, \omega) = \frac{u(k\sigma)v(k\sigma)}{\omega - \epsilon_+(k\sigma)} - \frac{u(k\sigma)v(k\sigma)}{\omega - \epsilon_-(k\sigma)} = G_0^{ba}(k\sigma, \omega) \quad (38)$$

$$G_0^{bb}(k\sigma, \omega) = \frac{v^2(k\sigma)}{\omega - \epsilon_+(k\sigma)} + \frac{u^2(k\sigma)}{\omega - \epsilon_-(k\sigma)} \quad (39)$$

where

$$u^2(k\sigma) = 1/2(1 - z_\sigma \frac{K S_z}{R(k)}); v^2(k\sigma) = 1/2(1 + z_\sigma \frac{K S_z}{R(k)}); \quad (40)$$

$$\epsilon_\pm(k\sigma) = \pm R(k) = ((\epsilon^{ab}(k))^2 + K^2 S_z^2)^{1/2} \quad (41)$$

the simplest assumption is that each sublattice is s.c. and $\epsilon^{\alpha\alpha}(k) = 0(\alpha = a, b)$. In spite that we have worked in the GFs formalism, our expressions (37)-(39) are in accordance with the results of the Bogolubov (u,v)-transformation for fermions, but, of course, the present derivation is more general.

The mass operator M in Dyson equation (34), which describes hole-magnon scattering processes, is given by as a "proper" part [35] of the irreducible matrix GF of higher order

$$M(k\sigma, \omega) = \begin{pmatrix} \langle\langle A(k\sigma, a) | A^+(k\sigma, a) \rangle\rangle^{(ir)} & \langle\langle A(k\sigma, a) | A^+(k\sigma, b) \rangle\rangle^{(ir)} \\ \langle\langle A(k\sigma, b) | A^+(k\sigma, a) \rangle\rangle^{(ir)} & \langle\langle A(k\sigma, b) | A^+(k\sigma, b) \rangle\rangle^{(ir)} \end{pmatrix} \quad (42)$$

To find the renormalization of the spectra $\epsilon_\pm(k\sigma)$ and the damping of the quasiparticles it is necessary to determine the self-energy for each type of excitations. From the formal solution (8) one immediately obtain

$$G_\pm(k\sigma) = (\omega - \epsilon_\pm(k\sigma) - \Sigma^\pm(k\sigma, \omega))^{-1} \quad (43)$$

Here the self-energy operator is given by

$$\Sigma^{\pm}(k\sigma, \omega) = A^{\pm} M^{aa} \pm B(M^{ab} + M^{ba}) + A^{\mp} M^{bb} \quad (44)$$

where

$$A^{\pm} = \begin{pmatrix} u^2(k\sigma) \\ v^2(k\sigma) \end{pmatrix}$$

$$B = u(k\sigma)v(k\sigma)$$

Equations (43) determines the quasiparticle spectrum with damping ($\omega = E - i\Gamma$) for the hole in the AFM background. Contrary to the simplified calculations of the hole GF in Section 4, the self-energy (42) is proportional to K^2 but not t^2 (c.f.eqn. (19))

$$M^{\alpha\beta}(k\sigma, \omega) = N^{-1} K^2 \sum_q \int_{-\infty}^{+\infty} d\omega_1 d\omega_2 \frac{1 + N(\omega_1) - n(\omega_2)}{\omega - \omega_1 - \omega_2} \quad (45)$$

$$(F_{\alpha\beta}^{\sigma,-\sigma}(q, \omega_1) g_{\alpha\beta}(k + q - \sigma, \omega_2) + F_{\alpha\beta}^{z\sigma}(q, \omega_1) g_{\alpha\beta}(k + q, \omega_2))$$

Here functions $N(\omega)$ and $n(\omega)$ are Bose and Fermi distributions, respectively, and the following notations have been used for spectral intensities

$$F_{\alpha\beta}^{ij}(q, \omega) = -\frac{1}{\pi} \text{Im} \langle\langle S_{q\alpha}^i | S_{-q\beta}^j \rangle\rangle_{\omega} \quad (46)$$

$$g_{\alpha\beta}(k\sigma, \omega) = -\frac{1}{\pi} \text{Im} \langle\langle a_{\alpha}(k\sigma) | a_{\beta}^{\dagger}(k\sigma) \rangle\rangle_{\omega}; \quad i, j = (+, -, z).$$

The equations (45) and (34) forms the self-consistent set of equations for the determining of the GF (31). It need hardly be remarked that the advantages of the present formulation permits:

- i) to make much more exact statements about interacting hole-spin system
- ii) to calculate in controlled manner beyond the Hartree-Fock approximation,
- iii) with IGF method we can make a one-to-one correspondence between each complete set of contractions arising in each term of diagrammatic expansion(c.f. [48], [49]).

Coupled equations (45) and (34) can be solved analytically by suitable iteration procedure. In principle, we can use, in the right-hand side of (45) any workable first iteration step for of the relevant GFs and find a solution by repeated iteration. It is most convenient to choose as the first iteration step the simplest two-pole expressions, corresponding to the GF structure for a mean field, in the following form

$$g_{\alpha\beta}(k\sigma, \omega) = R_+ \delta(\omega - E_+(k\sigma)) + R_- \delta(\omega - E_-(k\sigma)) \quad (47)$$

where R_{\pm} are the certain coefficients depending on $u(k\sigma)$ and $v(k\sigma)$. The magnetic excitation spectrum corresponds to the frequency poles of the GFs (29). In view of the discussion elsewhere of the spin dynamics of the present model, we shall content ourselves with the simplest initial approximation for the spin GF occurring in (45) (c.f. [39])

$$\frac{1}{2z_{\sigma} S_z} F_{\alpha\beta}^{\sigma-\sigma}(q, \omega) = L_+ \delta(\omega - z_{\sigma}\omega_q) - L_- \delta(\omega + z_{\sigma}\omega_q) \quad (48)$$

Here ω_q is the energy of the antiferromagnetic magnons and L_{\pm} are the certain coefficients (see [39]). We are now in a position to find an explicit solution of coupled equations obtained so far. This is achieved by using (47) and (48) in the right-hand-side of (45). Then the hole self-energy in 2D quantum antiferromagnet for the low-energy quasiparticle band $E_-(k\sigma)$ is

$$\begin{aligned} \Sigma^-(k\sigma, \omega) = & \frac{K^2 S_z}{2N} \sum_q C_-^2 \left(\frac{1 + N(\omega_q) - n(E_-(k-q))}{\omega - \omega_q - E_-(k-q)} + \frac{N(\omega) + n(E_-(k+q))}{\omega + \omega_q - E_-(k+q)} \right) \\ & + \frac{2K^2 S_z^2}{N} \sum_{qp} D_-^2 \frac{N(\omega_{q+p})(1 + N(\omega_q)) + n(E_-(k+p))(N(\omega_q) - N(\omega_{q+p}))}{\omega + \omega_{q+p} - \omega_q - E_-(k+p)} \end{aligned} \quad (49)$$

Here we have used the notations

$$C_-^2 = (U_q + V_q)^2; \quad D_-^2 = (U_q U_{q+p} - V_q V_{q+p})^2$$

where the coefficients U_q and V_q appears as a results of explicit calculation of the mean-field magnon GF [39].

A very remarkable feature of this result is that our expression (49) accounts for the hole-magnon inelastic scattering processes with the participation of one or two magnons. It will be important for the consideration of Cooper pairing processes as we will show elsewhere. The self-energy representation in a self-consistent form (45) provide a possibility to model the relevant spin dynamics by selecting spin-diagonal or spin-off-diagonal coupling as a dominating or having different characteristic frequency scales. As a workable pattern, we consider now the static trial approximation for the correlation functions of the magnon subsystem [39] in the expression (45). Then the following expression is readily obtained

$$\begin{aligned} M^{\alpha\beta}(k\sigma, \omega) = & \frac{K^2}{N} \sum_q \int_{-\infty}^{+\infty} \frac{d\omega'}{\omega - \omega'} \left(\langle S_{-q\beta}^{-\sigma} S_{q\alpha}^{\sigma} \rangle g_{\alpha\beta}(k+q-\sigma, \omega') \right. \\ & \left. + \langle (S_{-q\beta}^z)^{ir} (S_{q\alpha}^z)^{ir} \rangle g_{\alpha\beta}(k+q\sigma, \omega') \right) \end{aligned} \quad (50)$$

Taking into account (49) we find the following approximative form

$$\Sigma^-(k\sigma, \omega) \approx \frac{K^2}{2N} \sum_q \frac{\chi^{-+}(q) + \chi^{z,z}(q)}{\omega - E_-(k+q)} (1 - \gamma_1(q)) \quad (51)$$

The dynamics of spin-1/2 Heisenberg antiferromagnet with nearest-neighbor exchange constant J , on a two-dimensional square lattice deserves a more detailed discussion. This will be done in the near future.

It should be noted, however, that in order to make this kind of study valuable as one of the directions to studying the mechanism of HTSC the binding of quasiparticles must be taking into account. This very important problem [46],[48],[54] deserves the separate consideration. In spite of formal analogy of the our model (21) with that of a Kondo lattice, the physics are different(c.f. [55]). There is a dense system of spins interacting with a smaller concentration of holes. As many authors have mentioned, for the obtaining the magnon exchange mediated superconductivity (of the non-s-wave character most

probably) the suitable effective interactions between two fermions, which is relevant for the case, is two-magnon exchange-type of interaction. Whese the fermion-magnon bound state formation has to be suppressed or not for promotion of the appearance of the superconductivity is not quite clear problem [56]. This question is in close relation with the right definition of the magnon vacuum for the case when $K \neq 0$.

In this Section we has considered the simplest possibility, assuming that dispersion relation $\epsilon^{\alpha\alpha}(k) = 0$ ($\alpha = a, b$). In paper [57] a model of hole carriers in an antiferromagnetic background has been discussed, which explains many specific properties of cuprates. The effect of strong correlations is contained in the dispersion relation of the holes. The main assumption is that the influence of antiferromagnetism and strong correlations is contained in the special dispersion relation, $\epsilon(k)$, which was obtained using a numerical method. The best fit corresponds to[57]

$$\epsilon(k) = -1.255 + 0.34 \cos k_x \cos k_y + 0.13(\cos 2k_x + \cos 2k_y) \quad (52)$$

As a result, the main effective contribution to $\epsilon(k)$ arises from hole hopping between sites belonging to the same sublattice, to avoid distorting the antiferromagnetic background. Our analytical approach is similar in spirit to numerical approach of the paper[57]. Our IGF method is essentially self-consistent, i.e. do not depends on the special initial form for the hole propagator. For the self-consistent calculation by iteration of the self-energy (45) we can take as the fist iteration step the expression (47) with the dispersion relation (52). This must be done for the calculation mean-field GF (35) and dispersion relation (41) too. This approach will be discussed elsewhere.

7 Conclusions

In summary, in this paper we have presented calculations for normal phase of HTSC, which are describable in terms of the spin-fermion model. We have characterized the true quasiparticle nature of the carriers and the role of magnetic correlations. It was shown that the physics of spin-fermion model can be understood in terms of competition between antiferromagnetic order on the CuO_2 -plane preferred by superexchange J and the itinerant motion of carriers. It appears plausible that similar arguments apply to calculation of the static hole states for $t - J$ model since the latter are intimately related to that of spin-fermion model. It is thus highly advisable to investigate comparative hole quasiparticle dynamics of the both models. In the present paper we do not presented all the details as regards for different possibilities of the definition of the relevant generalized mean fields in this formalism. Carrying this procedure to other possibilities leads to a much more rich set of solutions for the spin-fermion model. In the light of this situation it is clearly of interest to explore in details how the hole motion relate with that of the Zhang-Rice singlet and other composit "carriers" in the framework of the present formalism. Considering that the carrier-doping results in the HTSC for the realistic parameters range $t \gg J, K$, corresponding the situation in oxide superconductors, the careful examination of the collective behaviour of the carriers for a moderately doped system must be performed [58]. It seems that this behaviour can be very different from that of single hole

case. The problem of the coexistence of the suitable Fermi-surface of mobile fermions and the antiferromagnetic long range or short range order has to be clarified. The volume of the Fermi surface is an important problem, which was discussed recently[59]. The question was considered how to model doped cuprates. Should one model them by a system of quasi-particles which corresponds to the doped holes and populate the dispersion relation calculated for a single hole (rigid-band approximation). This is very intriguing problem, which deserves the careful analysis. Finally, in the present paper we have considered the simplified spin-fermion model, taking into account a Kondo-like spin coupling K between the oxygen hole and two nearest copper spins, arising from the strong d-p hybridization of the three-band extended Hubbard model [2]-[5]. However hybridization induces effective spin-preserving hopping and spin-exchanging hopping terms also, implicitly taking into account the charge-transfer processes. The picture of the charge-transfer processes is modified greatly by taking into account the long-range screened Coulomb interaction within d-p model[60]. Work is in progress to refine the present approach for calculating of two-hole dynamics and the binding of quasiparticles for more general models.

References

- [1] *Correlation Effects in Low-Dimensional Electron Systems*, edited by A.Okiji and N.Kawakami (Springer-Verlag,Berlin,1994)
- [2] A.L.Kuzemsky, in *Superconductivity and Strongly Correlated Electron Systems*, edited by C.Noce, A.Romano and G.Scarpetta (World Scientific, Singapoure, 1994), p.346
- [3] *Correlated Electron Systems*, edited by V.J.Emery (World Scientific, Singapoure, 1993)
- [4] E.Dagotto, *Rev.Mod.Phys.* **66**, 763 (1994)
- [5] Yu Lu, in *Recent Progress in Many-Body Theories*, edited by T.L.Ainsworth et al (Plenum Press, New York, 1992), Vol.3, p.157
- [6] E.Manousakis, *Rev.Mod.Phys.* **63**, 1 (1991)
- [7] A.R.Bishop et al, *Phys.Rev.Lett.* **61**, 2709 (1988)
- [8] S.Sachdev and R.Shankar, *Phys.Rev.* **B38**, 826 (1988)
- [9] R.Joynt, *Phys.Rev.* **B37**, 7979 (1988)
- [10] S.Schmitt-Rink, C.M.Varma and A.Ruckenstein, *Phys.Rev.Lett.* **60**, 2793 (1988)
- [11] W.Brenig and K.Becker, *Z.Physik*,**B76**, 473 (1989)
- [12] R.Shankar, *Phys.Rev.Lett.* **63**, 203 (1989)
- [13] Z.B.Su, Y.M.Li, W.J.Lai and L.Yu. *Phys.Rev.Lett.* **63**, 1318 (1989) ;
Int.J.Mod.Phys. **B3**, 1913 (1989)

- [14] C.L.Kane, P.A.Lee and N.Read, Phys.Rev. **B39**, 6880 (1989)
- [15] R.Eder and K.Becker, Z.Physik, **B78**, 219 (1990)
- [16] R.Eder and K.Becker, Z.Physik, **B79**, 333 (1990)
- [17] Yang Chen, Phys.Rev. **B41**, 9455 (1990)
- [18] Yang Chen, Phys.Rev. **B42**, 6769 (1992)
- [19] J.H.Hu, C.S.Ting and T.K.Lee, Phys.Rev. **B43**, 8733 (1990)
- [20] I.Ichinose and T. Matsui, Phys.Rev. **B44**, 7654 (1991)
- [21] G.Martinez and P.Horsch, Phys.Rev. **B44**, 2414 (1991)
- [22] A.Auerbach and B.E.Larson, Phys.Rev. **B43**, 7800 (1991)
- [23] I.Ichinose and T.Matsui, Phys.Rev. **B45**, 9976 (1992);
Nuclear Physics, **B441**[FS], 483 (1995)
- [24] D.Poiblan, H.J.Schultz and T.Ziman, Phys.Rev. **B46**, 6435 (1992)
- [25] H.Q.Ding, Physica **C203**, 91 (1992)
- [26] Y.M.Li, W.J.Lai, Z.B.Su and L. Yu, Phys.Rev. **B47**, 7938 (1993)
- [27] K.Miura, Physica **C208**, 297 (1993)
- [28] Q.F.Zhong, S.Sorella and A.Parola, Phys.Rev. **B49**, 6408 (1994);
Q.F.Zhong and S.Sorella, Phys.Rev. **B51**, 16135 (1995)
- [29] J.Inoue, K.Iiyama, S.Kobayashi and S.Maekawa, Phys.Rev. **B49**, 6213 (1994)
- [30] M.Acquarone and M.Pausico, Acta Physica Pol., **84**, 101 (1993);
J.R.Schrieffer, Solid State Commun.**92**,129 (1994)
- [31] Y.C.Chen, Phys. Lett. **A173**, 329 (1993)
- [32] T.Nishino, J.Phys.Soc.Jpn. **59**, 4376 (1990)
- [33] I.Kanazawa, in *The Physics and Chemistry of Oxide Superconductors*, edited by Y.Iye and H.Yasuoka (Springer-Verlag, Berlin, 1992),p.481
- [34] A.L.Kuzemsky, Doklady Acad.Nauk SSSR **309**, 323 (1989)
- [35] A.L.Kuzemsky, Nuovo Cimento, **B109**, 829 (1994)
- [36] A.L.Kuzemsky, Preprint ICTP IC/94/292, Trieste, 1994
- [37] D.Marvakov, J.Vlahov and A.L.Kuzemsky, J.Phys.:**C18**, 2871 (1985)

- [38] D.Marvakov, A.L.Kuzemsky and J.Vlahov, *Physica* B**138**, 129 (1986)
- [39] A.L.Kuzemsky and D.Marvakov, *Theor.Math.Phys.* **83**, 147 (1990)
- [40] A.L.Kuzemsky, *Phys.Lett.* A**153**, 466 (1991);
Intern.J.of Modern Phys. Ser.B (1996)
- [41] A.L.Kuzemsky, J.C.Parlebas and H.Beck, *Physica* A**198**, 606 (1993)
- [42] A.L.Kuzemsky, *Theor.Math.Phys.* **36**, 208 (1978)
- [43] A.L.Kuzemsky, *Dynamics of Highly Correlated Fermions on a Lattice*, Abstracts of the 19th IUPAP Intern. Conf. on Statistical Physics, Xiamen, (1995), p.10
- [44] S.Doniach and E.Sondheimer, *Green's Functions for Solid State Physicist* (Addison-Wesley, N.Y. 1974)
- [45] C.T.Rieck, W.A.Little, J.Ruvalds and A.Virostek, *Solid State Comm.* **88**, 395 (1993);
R.Hlubina and T.M.Rice, *Phys.Rev.* B**51**, 9253 (1995)
- [46] P.Prelovsek, *Phys.Lett.* A**126**, 287 (1988);
A.Ramsak and P.Prelovsek, *Helvetica Physica Acta*, **65**, 446 (1992)
- [47] S.Kurihara, *Phys.Rev.* B**39**, 6600 (1989)
- [48] N.Furukawa and M.Imada, *J.Phys.Soc.Jpn.* **59**, 1771 (1990)
- [49] J.Inoue and S.Maekawa, *J.Phys.Soc.Jpn.* **59**, 2110 (1990)
- [50] N.Mitani and S.Kurihara, *Physica* C**206**, 13 (1993)
- [51] H.Shimahara, *J.Phys.Soc.Jpn.* **62**, 1317 (1993)
- [52] N.Mitani and S.Kurihara, *Phys.Lett.* A**184**, 374 (1994)
- [53] H.Shimahara, *J.Phys.Soc.Jpn.* **63**, 374 (1994);
M.Hamada and H.Shimahara, *Phys.Rev.* B**51**, 3027 (1995)
- [54] D.Poilblanc, J.Riera and E.Dagotto, *Phys.Rev.* B**49**, 12318 (1994)
- [55] Y.Okimoto et al, *Phys.Rev.Lett.* **75**, 109 (1995)
- [56] M.Kang and O.Nagai, *JMMM*, **140-144**, 1937 (1995)
- [57] E.Dagotto, A.Nazarenko and M.Boninsegni, *Phys.Rev.Lett.* **73**, 728 (1994)
- [58] E.S.Heeb and T.M.Rice, *Europhys.Lett.* **27**, 673 (1994)
- [59] R.Eder, Y.Ohta and T.Shimozato, *Phys.Rev.* B**50**, 3350 (1994)
- [60] J.Riera and E.Dagotto, *Phys.Rev.* B**50**, 3215 (1994)

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Куземский А.Л., Марваков Д.
Динамика каррионов в спин-фермионной модели

E17-96-99

Изучался спектр квазичастичных дырочных возбуждений (каррионов) и роль магнитных корреляций в рамках спин-фермионной (Кондо — Гайзенберга) модели с помощью метода уравнений движения. Динамика квазичастичных дырочных возбуждений рассматривалась в сравнении с динамикой t - J модели с тем, чтобы наиболее отчетливо выявить, как одно- и двухмагнонные процессы рассеяния определяют подлинную природу носителей в высокотемпературных сверхпроводниках. Для модели Кондо — Гайзенберга на основе уравнения Дайсона, т.е. за рамками приближения среднего поля, было найдено новое выражение для массового оператора с учетом процессов неупругого двухмагнонного рассеяния, которые могут играть роль в формировании сверхпроводящего состояния.

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Kuzemsky A.L., Marvakov D.
Dynamics of Carriers in the Spin-Fermion Model

E17-96-99

The spectrum of hole quasiparticles (carriers) and the role of magnetic correlations has been considered in the framework of spin-fermion (Kondo-Heisenberg) model by means of the equation-of-motion method. The hole quasiparticle dynamics has been discussed for t - J model and compared with that of spin-fermion model to determine how the one- and two-magnon processes define the true nature of carriers in HTSC. For this Kondo-Heisenberg-type model it was clearly pointed out on the self-energy level, beyond Hartree-Fock approximation, that two-magnon processes can play a role for the formation of the superconducting state.

The investigation has been performed at the Bogoliubov Laboratory of Theoretical Physics, JINR.

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