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METHODS
OF THEORETICAL PHYSICS

Formation of Exotic States in the *s–d* Exchange and *t–J* Models

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Different scenarios of the implementation of the two-band model in systems of strongly correlated electrons, including frustrated magnetic systems, high-temperature superconductors, and Kondo lattices, are considered. The interaction of current carriers with magnetic moments in the representations of pseudofermions or Schwinger bosons describing the spinon excitations is studied on the basis of the derived Hamiltonians of the *s–d* exchange and *t–J* models within the formalism of many-electron Hubbard X operators.

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1. INTRODUCTION

Unusual excitations and exotic states in strongly correlated solid states and other condensed media, e.g., different types of spin liquids and states with topological and quantum orders, are currently under active investigation [1]. They are usually described within many-electron models. The simplest of them is the one-band *t–J* model, in which strong single-site correlations and the exchange interaction between localized spins are taken into account. Though it makes it possible to consider a series of exotic phases and is successively applied to physics of cuprates (basic systems for high-temperature superconductors (HTSCs)) [2, 3], the corresponding approximations are difficult to control owing to the absence of a small parameter: the simplicity of a model often does not provide the convenience of the theoretical study.

On the other hand, in physics of magnetic semiconductors, heavy fermion systems, and Kondo lattices, as a rule, one uses the two-band *s–d*(*f*) exchange model, in which subsystems of current carriers and local magnetic moments are separated initially; in addition, the model is convenient because it has a semiclassical small parameter. The idea of such separation acquires a new meaning in current field-theoretical approaches, where the formation of exotic phases and particles with unusual statistics is considered. It is assumed that such states are implemented in insulating and conducting f- and d-systems (here, in addition to cuprates, frustrated band magnets of the YMn_2 type can be mentioned [4]).

In this work, we show that the usage of the two-band (in particular, *s–d* exchange) model as the more general one makes it possible to clarify a series of moments in the physical understanding of the state of spin liquid. In addition, we demonstrate the description of exotic excitations in terms of many-electron Hubbard X operators.

2. MODEL HAMILTONIAN

The *t–J* model, which is the Hubbard model with the infinite single-site repulsion $U \to \infty$ and allowance for the Heisenberg exchange, is widely used at the theoretical consideration of strongly correlated compounds (e.g., copper–oxygen HTSC). Its Hamiltonian in the many-electron representation of Hubbard operators $X(\Gamma,\Gamma') = |\Gamma\rangle\langle\Gamma'|$ has the form

$$H = \sum_{ij\sigma} t_{ij} X_i(0\sigma) X_j(\sigma 0) + H_d, \quad H_d = \sum_{ij} J_{ij}\mathbf{S}_i\mathbf{S}_j, \tag{1}$$

where t_{ij} are transfer integrals and J_{ij} are exchange parameters.

The model (1) describes the interaction of current carriers with local moments. To demonstrate explicitly the separation of these degrees of freedom, we note its equivalence to the *s–d* exchange model with the exchange parameter $I \to -\infty$. In fact, after passing to the many-electron representation, the Hamiltonian of the latter is written as [5, 6]

$$H = \sum_{ij\sigma} t_{ij} g^\dagger_{i\sigma} g_{j\sigma} + H_d, \tag{2}$$

$$g^\dagger_{i\sigma} = \sum_M C^{S-1/2,M+\sigma}_{SM;1/2,\sigma} X_i(S-1/2, M+\sigma; SM), \tag{3}$$

where

$$C^{S-1/2,M+\sigma}_{SM;1/2,\sigma} = (S - 2\sigma M)^{1/2}/(2S+1)^{1/2} \tag{4}$$

are the Clebsch–Gordan coefficients for the coupling of spins S and 1/2. It is easy to see that the Hamiltonian (2) at $S = 1/2$ coincides with (1) with the trivial renormalization: $t_{\mathbf{k}}$ is replaced in (2) by $2t_{\mathbf{k}}$ (the factor 2 appears owing to the equivalence of transitions of electrons with both opposite spins in the Hubbard model).

The standard representation of auxiliary (slave) bosons introduced by Anderson [2] has the form

$$X_i(\sigma,0) = f_{i\sigma}^{\dagger}e_i. \tag{5}$$

Here, e_i are annihilation operators for charged spinless bosons (holons) and $f_{i\sigma}^{\dagger}$ are creation operators for neutral fermions (spinons). It is also possible to use the representation of auxiliary fermions

$$X_i(\sigma,0) = b_{i\sigma}^{\dagger}e_i, \tag{6}$$

where now e_i and $b_{i\sigma}^{\dagger}$ are Fermi and Bose (Schwinger) operators, respectively. However, we will use directly the X operators, introducing spinons only for the localized subsystem.

In turn, the Hamiltonian (2) can be expressed in terms of Fermi operators and operators of localized spins. Using the representation of Hubbard operators in terms of many-electron operators of the creation of electron configurations $A_{\Gamma}^{\dagger}$ [5, 6],

$$X(\Gamma,\Gamma') = A_{\Gamma}^{\dagger}\prod_{\sigma}(1-n_{\sigma})A_{\Gamma'}, \quad n_{\sigma} = c_{\sigma}^{\dagger}c_{\sigma}, \tag{7}$$

and the relation

$$A_{S-1/2,\mu}^{\dagger} = \sum_{M\sigma}C_{SM,1/2\sigma}^{S-1/2,\mu}c_{\sigma}^{\dagger}A_{SM}^{\dagger}, \tag{8}$$

it is possible to separate the operators of conduction electrons on the space of singly occupied states from X operators. Identically transforming the product of Clebsch–Gordan coefficients, we find

$$g_{i\sigma}^{\dagger} = \sum_{\sigma'}c_{i\sigma'}^{\dagger}(1-n_{i,-\sigma'})\frac{S\delta_{\sigma\sigma'} - (\mathbf{S}_i\boldsymbol{\sigma}_{\sigma'\sigma})}{2S+1}. \tag{9}$$

Further, the usage of the properties of Pauli matrices gives

$$\begin{aligned} H &= \frac{1}{(2S+1)^2} \\ &\times \sum_{ij\sigma\sigma'}t_{ij}\{(S^2 + \mathbf{S}_i\mathbf{S}_j)\delta_{\sigma\sigma'} - S(\mathbf{S}_i + \mathbf{S}_j)\boldsymbol{\sigma}_{\sigma\sigma'} \\ &+ i\boldsymbol{\sigma}_{\sigma\sigma'}[\mathbf{S}_i\times\mathbf{S}_j]\}c_{i\sigma}^{\dagger}(1-n_{i,-\sigma})(1-n_{j,-\sigma'})c_{j\sigma'} + H_d. \end{aligned} \tag{10}$$

Such representation of the Hamiltonian (of course, also valid in the t–J model) was obtained for the first time in [5, 6]. Later, it was used in [7] as applied to the phase diagram of HTSC cuprates as "new formulation of the t–J model;" a somewhat different interpretation was given: the arising electron states were called dopons.

The transition to the s–d exchange model with strong correlations makes it possible to naturally expand the physical space and at the same time (unlike the consideration of the t–J model [7]) remove the nonphysical state owing to the condition $I \to -\infty$. However, the generalization to the case of the s–d exchange model with finite I is also possible:

$$H = \sum_{\mathbf{k}\sigma}t_{\mathbf{k}}c_{\mathbf{k}\sigma}^{\dagger}c_{\mathbf{k}\sigma} - I\sum_{i\alpha\beta}\mathbf{S}_i\boldsymbol{\sigma}_{\alpha\beta}c_{i\alpha}^{\dagger}c_{i\beta} + H_d, \tag{11}$$

which, in particular, describes Kondo lattices.

Terms linear in spin operators in Eq. (10) provide the possibility of the effective hybridization of electrons with spinons, as in Kondo lattices. Terms containing vector products, though they disappear for simple spin configurations, describe the anisotropic scattering of electrons. Thereby, the Hamiltonian (10) can be useful in the consideration of states with anomalous "chiral" order parameters of kinetic phenomena in narrow bands, e.g., the anomalous Hall effect (see, e.g., [8]).

3. CASE OF A SINGLE CURRENT CARRIER

In model (11), the expression for the energy of the electron in the second-order perturbation theory in the case of the empty conduction band has the form

$$\Sigma_{\mathbf{k}}^{(2)}(E) = \Phi_{\mathbf{k}}(E) = I^2\sum_{\mathbf{q}}\int\frac{K_{\mathbf{q}}(\omega)d\omega}{E - t_{\mathbf{k+q}} + \omega}, \tag{12}$$

where $K_{\mathbf{q}}(\omega)$ is the spin spectral function. To find it, we consider different spinon representations for localized spins.

In the self-consistent spin-wave theory, the representation of Schwinger bosons is used [9]:

$$\mathbf{S}_i = \frac{1}{2}\sum_{\sigma\sigma'}b_{i\sigma}^{\dagger}\boldsymbol{\sigma}_{\sigma\sigma'}b_{i\sigma'}, \tag{13}$$

or that of Dyson–Maleev [10]. This makes it possible to describe the quantum disordered state (spin liquid) and the magnetically ordered phase with the wave vector $\mathbf{Q}$, the latter being considered as the boson condensate (at low temperatures, the state close to the condensate arises in the regions with the exponentially large correlation length, which is described analogously; i.e., the "effective" magnetization of the sublattice $\bar{S}_{\mathrm{eff}}(T)$ hardly changes [11]). After the separation of condensate contributions (extra factors of 3/2 appear in them when using the Schwinger bosons, which we omit), we find

$$\begin{aligned} K_{\mathbf{q}}(\omega) &= \bar{S}_{\mathrm{eff}}^2\delta(\omega)\delta_{\mathbf{qQ}} + \bar{S}_{\mathrm{eff}}(u_{\mathbf{q}} - v_{\mathbf{q}})^2\delta(\omega + \omega_{\mathbf{q}}) \\ &+ \sum_{\mathbf{p}}(u_{\mathbf{p-q}}v_{\mathbf{p}} - v_{\mathbf{p-q}}u_{\mathbf{p}})^2\delta(\omega + \omega_{\mathbf{p-q}} + \omega_{\mathbf{p}}). \end{aligned} \tag{14}$$

The first term in (14) leads to the formation of the antiferromagnetic gap and will be ignored (this is justified near the band bottom). The second term describes the interaction with spin waves (it is absent in the quantum disordered state, since a gap arises in the spectrum of spinons), and the third term describes the interaction with the individual spinon excitations.

In the state of resonating valence bonds, the Hamiltonian of the d-subsystem is written in the representation of pseudofermions analogous to (13) as in [3, 12]:

$$H_d = \sum_{\mathbf{k}\sigma}(B_\mathbf{k} f^\dagger_{\mathbf{k}\sigma} f_{\mathbf{k}\sigma} + \Delta_\mathbf{k} f_{\mathbf{k}\sigma} f_{-\mathbf{k}-\sigma} + \text{H.c.}), \tag{15}$$

where $B_\mathbf{k} \sim J_\mathbf{k}$.

The corresponding spectral density is obtained in the approximation of noninteracting Fermi spinons and is analogous to the last term in Eq. (14):

$$K_\mathbf{q}(\omega) = \sum_\mathbf{k}(u_{\mathbf{k}-\mathbf{q}} v_\mathbf{k} - v_{\mathbf{k}-\mathbf{q}} u_\mathbf{k})^2 \delta(\omega + E_{\mathbf{k}-\mathbf{q}} + E_\mathbf{k}), \tag{16}$$

where the spectrum $E_\mathbf{k} = (B^2_\mathbf{k} + \Delta^2_\mathbf{k})^{1/2}$ and the coefficients of the Bogoliubov transformation (now Fermi type) are obtained during the diagonalization of (15).

In the antiferromagnetic and quantum disordered states and in the resonating valence bond state, the combination of coefficients of the u–v transformation in $K_\mathbf{q}(\omega)$ becomes zero at $q \to 0$.

We consider the structure of the electron spectrum near the band bottom in the case of a single current carrier. In the self-consistent approximation, replacing energy denominators by exact Green's functions, we obtain the integral expression

$$\Phi_\mathbf{k}(E) = I^2 \sum_\mathbf{q} \int K_\mathbf{q}(\omega) G_{\mathbf{k}+\mathbf{q}}(E + \omega) d\omega. \tag{17}$$

To solve Eq. (17), it is possible to apply the approximation of the "dominating pole" [11, 12]:

$$G_\mathbf{k}(E) = \frac{Z_\mathbf{k}}{E - \tilde{E}_\mathbf{k}} + G_\text{inc}(\mathbf{k}, E), \tag{18}$$

where G_inc is the incoherent contribution to the Green's function and

$$Z_\mathbf{k} = \left(1 - \frac{\partial}{\partial E}\text{Re}\Sigma_\mathbf{k}(E)\right)^{-1}_{E=\tilde{E}_\mathbf{k}} \tag{19}$$

is the residue at the pole near the band bottom corresponding to the spectrum of new quasiparticles $\tilde{E}_\mathbf{k}$.

Substituting Eq. (18) into Eq. (17) and integrating over q, we obtain the estimate in the two-dimensional case:

$$Z^{-1} - 1 \sim I^2/|Jt|. \tag{20}$$

Thus, with the increase in $|I|$, the spectral weight transfers into the incoherent contribution and undamped quasiparticles become heavy, so that, at $I^2 \gg J|t|$, the effective mass is $m^*/m = Z^{-1} \gg 1$. In the three-dimensional case, the divergence is weaker, and corrections to the residue contain only the logarithmic factor: $Z^{-1} - 1 \sim I^2 S \ln|t/JS|$ [11].

In the case of narrow bands ($I \to -\infty$), we consider the Green's function of many-electron operators

$$G_{\mathbf{k}\sigma}(E) = \langle\langle g_{\mathbf{k}\sigma} | g^\dagger_{\mathbf{k}\sigma}\rangle\rangle_E. \tag{21}$$

The result of calculations with allowance for spin fluctuations [11] has the form

$$G_{\mathbf{k}\sigma}(E) = \Psi_\mathbf{k}(E)/[E - \Psi_\mathbf{k}(E) t_\mathbf{k}], \tag{22}$$

$$\Psi_\mathbf{k}(E) = \frac{S}{2S+1} + \sum_\mathbf{q} \frac{t_{\mathbf{k}+\mathbf{q}}}{(2S+1)^2} \times \int K_\mathbf{q}(\omega) \Psi^{-1}_{\mathbf{k}+\mathbf{q}}(E) G_{\mathbf{k}+\mathbf{q}}(E + \omega) d\omega. \tag{23}$$

As was noted in [12], the effect of the finite width of the bare band (the first term on the right-hand side of Eq. (23)) and details of the approximation are not important for the quasiparticle pole, though they are essential for the incoherent contribution. As a result, we find

$$Z^{-1} - 1 \sim \begin{cases} |t/JS| \\ \text{for two-dimensional case,} \\ S^{-1} \ln|t/JS| \\ \text{for three-dimensional case.} \end{cases} \tag{24}$$

Our approach considers physical excitations rather than auxiliary particles, i.e., holons (bosons or fermions) as in [12] (where it is also noted that the calculation of the boson Green's function is not quite physically consistent). Since the results (18) and (20) are determined by divergences at low momenta, they are also obtained in the spin-wave picture [11] and in both ways of the consideration of the quantum disordered state in terms of bosons and fermions. We will see below that a similar change of the statistics from the Bose to Fermi one also occurs in Kondo lattices.

The further development of the theory takes into account the interaction with the gauge field [3]; apparently, it is not too important in the case of the spin liquid of the Z_2 type, but is essential for $U(1)$.

4. CASE OF THE FINITE BAND FILLING

At the partial filling of the conduction band, we come to the situation of the Kondo lattice. If the Kondo temperature $T_\text{K} \sim \exp(1/2I\rho(E_\text{F}))$ (where $\rho(E)$ is the bare density of states) is much higher than the d–d exchange J, localized moments are screened by conduction electrons and the ground state of the heavy Fermi liquid appears. However, other exotic phases can also appear in the general case. If the d–d bonds are frustrated, the d moments can form the spin liquid, which does not violate the symmetry of the lattice Hamiltonian [3]. The deconfinement state arises at the boundary between the magnetic phase and the

Fermi liquid in the form of the algebraic spin liquid with the non-Fermi-liquid behavior and the separation of the charge and spin degrees of freedom [3]. The formation of the exotic disordered state can be achieved not only by the direct introduction of frustration into the spin subsystems but also by doping.

First, we discuss the results of perturbation theory [13–15]. The calculation of the magnetic susceptibility with allowance for spin dynamics leads to the result

$$\chi = \frac{S(S+1)}{3T} - \frac{4I^2}{3T}\sum_{\mathbf{pq}}\int K_{\mathbf{p}-\mathbf{q}}(\omega)\frac{n_{\mathbf{p}}(1-n_{\mathbf{q}})}{(t_{\mathbf{q}}-t_{\mathbf{p}}-\omega)^2}d\omega, \quad (25)$$

where the second term describes the screening of the moment and $n_{\mathbf{k}}$ are Fermi distribution functions.

The Kondo contribution to the imaginary part of the self-energy arising in the third-order perturbation theory has the form

$$\mathrm{Im}\Sigma^{(3)}_{\mathbf{k}}(E) = 2\pi I^3\rho(E)\int\sum_{\mathbf{q}}K_{\mathbf{q}}(\omega)\frac{n_{\mathbf{k}+\mathbf{q}}}{E-t_{\mathbf{k}+\mathbf{q}}-\omega}d\omega. \quad (26)$$

The usage of the corresponding spectral function makes it possible to take into account the cutoff of Kondo divergences and to develop the renormalization group theory of Kondo lattices analogously to [13, 14] not only in magnetic phases but also for states of the spin liquid type with the non-Fermi-liquid behavior.

For the description of the ground state (the strong coupling regime), it is possible to use the mean field theory in the representation of pseudofermions [16–19]. The most important effect here is the formation of the "large" Fermi surface, in which pseudofermions hybridizing with conduction electrons are involved. The condensation of Bose spinons (Schwinger bosons) means the formation of magnetism, and the condensation of the Higgs boson ($b_0 \sim \langle f^\dagger_{i\sigma}c_{i\sigma}\rangle$) in the Kondo phase means the formation of the Fermi liquid with a large Fermi surface, though secondary magnetic ordering is also possible in this phase [18, 19].

The formation of the spin liquid (an exotic Fermi liquid in the terminology of [18, 19]) is the intermediate regime: the same as the magnetic ordering, it suppresses the Kondo effect; therefore, the effective $|I|$ value is not renormalized to infinity, as takes place in the case of a single Kondo impurity. The s-electrons are weakly coupled to the d-spin liquid and form the "small" Fermi surface, which covers the volume determined only by the density of s-electrons.

In the case of narrow bands (the t–J model), doping is responsible for a series of complex effects, in particular, for the competition of ferro- and antiferromagnetism leading to the formation of helical or nonuniform magnetic structures; more exotic (including topological) states, the formation of the pseudogap are also possible [3].

The consideration of the spectrum of cuprates reveals nodal–antinodal dichotomy [3]: the nature of the spectrum differs in different regions of the Fermi surface. The spectrum is gapless near the nodal points $(\pm\pi/2, \pm\pi/2)$ (where the excitations are described as Dirac fermions) and has a gap near the antinodal point $(0, \pi)$.

In the mean field theory for the t–J model [7], the electron spectral weight originates from two bands: the low-energy spinon band and the high-energy electron band. The spectral weight from the spinon band is a sharp coherent peak. The broad spectral weight from the electron band corresponds to the incoherent background. The strong hybridization mixing between spinons and electrons described by the Hamiltonian (10) arises near the nodal point, and mixing is absent near the antinodal point. The Fermi surface is large or remains small, respectively. In essence, the described picture is close to the hybridization two-band model of Kondo lattices, where the separation of the localized and itinerant states appears.

On the other hand, the representation of Schwinger bosons was used in [20] to describe the state with a small Fermi surface (spin liquid of the Z_2 type) in the same model, though no separation of the coherent band analogous to that considered in Section 3 was performed (the corresponding perturbation theory in the many-electron representation was earlier developed in [11, 21]).

The approach of many-electron operators makes it possible to simultaneously consider both cases and take into account the change in the statistics of spinons at the quantum phase transition, introducing different spectral functions for collective excitations.

5. CONCLUSIONS

We see that the usage of the two-band model makes it possible to provide the general physical description of exotic states of strongly correlated systems.

In the case of the Hubbard model with the finite Coulomb repulsion, we deal with the problem of the formation of local magnetic moments. The presence of the "direct" Heisenberg exchange favors their appearance, so that the physical situation becomes close to the s–d exchange model (formally, the Coulomb term at one site can be written in the "exchange" form $-U\mathbf{s}_i\mathbf{s}_i$). The separation of contributions of the coherent (quasiparticle) and incoherent (non-quasiparticle) states is essential. The latter can be described most simply in the ferromagnetic phase, where they, however, arise only for the down spin projection, describing bound states of the carrier with the spin up and magnon [22, 23].

The representation of Schwinger bosons can be introduced not only in the t–J model [20] but also in the antiferromagnetic phase of the spin-fermion model, which is the modification of the single-band

Hubbard model with finite interaction [24]. Therefore, the exotic Fermi liquid is implemented in the latter model. The spin-Fermi model [25] used in the interpolation description of collective magnetism (the analogy of which with the s–d exchange model is described in [26]) also makes it possible to separate spin and electron degrees of freedom.

The "Kondo" peak on the Fermi level also appears in approximation of the dynamic mean field theory reducing the Hubbard model to the effective Anderson model [27]. It should be noted that, unlike the Hubbard model, where the Coulomb interaction leads to the destruction of the Fermi liquid state (the formation of Hubbard subbands with a small Fermi surface), the effect of the s–d exchange is the opposite: a heavy Fermi liquid and a large Fermi surface appear with the increase in $|I|$. The origin is that these interactions lead to different pairing types of electrons and spinons, diagonal and off-diagonal (hybridization).

The change in the statistics of spinons occurs at the quantum phase transition between two phases of the confinement: the magnetic phase and the phase with the large Fermi surface. Such a problem requires further studies. Here, supersymmetric representations may turn out to be useful (see, e.g., [28]).

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