Two-band model and RVB-type states: application to Kondo lattices, pyrochlores and Mn-based systems

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Abstract
An exotic fractionalized Fermi-liquid FL* theory of metallic systems, which combines resonant-valence-bond (RVB) state and the band of current carriers, is treated. An application of this theory to spin-liquid, antiferromagnetic and nearly antiferromagnetic systems is proposed with the use of various bosonic and fermionic representations, a comparison with perturbation theory in the s – d(f) exchange model being performed. The topological aspects including formation of the small Fermi surface are treated. In the case of narrow bands (strong correlations), the ground state is considered as a direct product of RVB and dopon or Weng’s fermion states. Examples of Kondo lattices, doped pyrochlores, and metallic β-Mn, YMn2, Y1−xScxMn2 systems are discussed, analogies with copper-oxide systems being treated.

Keywords: Kondo lattices; fractionalized Fermi liquid; spin liquid; specific heat; antiferromagnetism

1. Introduction

The resonant-valence-bond (RVB) theory was developed in the pioneering works by Anderson [1, 2], who considered for the superconducting cuprates the concept of spin-charge separation with introducing exotic quasiparticles – charged bosons (holons) and neutral fermions (spinons). Early treatment concerned uniform RVB state with T-linear specific heat in the inulating phase. However, later more complicated approaches were elaborated, the magnetic frustrations playing an important role, see the reviews [3, 4].

Moreover, to describe all the electron states of cuprates, a nodal–antinodal dichotomy is required [3]: the picture of the spectrum changes when passing the Fermi surface. Near the nodal points (±π/2, ±π/2), the spectrum is formed by gapless Dirac quasiparticles, but has a gap at the antinodal point (0, π). Near a nodal point (but not near the antinodal one), there occurs a mixing between auxiliary spinons and current carriers (dopons, according to the treatment in Ref. [5]) owing to effective hybridization. This picture is close in another two-band situation – in the Kondo lattices. Here, the localized and itinerant electron states are mixed in the mean-field approach including the d(f)-pseudofermions, so that the pseudofermions take part in the Fermi surface.

Besides cuprates, anomalous behavior occurs in metallic systems which demonstrate both the Kondo effect and magnetic frustrations, especially in anomalous (Kondo-lattice and heavy-fermion) f-systems. They can possess reduced antiferromagnetic (AFM) moment or be near the quantum critical point – at or near the magnetic instability (see [6, 7, 8, 9]).

As a result of competition between intersite magnetic interactions and Kondo effect (screening of magnetic moments owing to resonance scattering), and their mutual renormalization, a unique energy and temperature scale should form in the strong-coupling regime – the Kondo temperature TK [6]. Unlike the crossover scenario in the case of one Kondo impurity, we can have in the Kondo lattices true phase transitions with participation of magnetic ordering. In the presence of magnetic frustrations, the situation becomes still more complicated since we have one more tuning parameter owing to the frustrations. Various scenarios of the ground state formation in such Kondo lattices were proposed, see [6, 10, 11].

A similar situation occurs also in some d-systems (early examples of a spin-liquid-like behavior in systems with spin and charge degrees of freedom were considered in Refs. [12, 13]), an “old” RVB theory [11] being applied. In particular, some Mn-based compounds demonstrate giant γT-linear specific heat or even non-Fermi-liquid behavior [14, 15, 16]. Usually the anomalous properties of metallic frustrated f-systems are treated within the Kondo-lattice theory and of d-systems within Moriya’s itinerant spin-fluctuation magnetism [17]. However, the picture of weak itinerant magnetism is hardly well suited in the situation with large Mn magnetic moments.

The most important and interesting effect of the frustrations is disordering of local moments, so that only partial delocalization of electron states, unlike standard Kondo lattices. Thus the system naturally described in the two-band picture including localized and itinerant degrees of freedom. The volume of the Fermi surface is determined by conduction electrons only (a so-called small Fermi surface). In the absence of increasing the unit cell (e.g., doubling which occurs in the case of antiferromagnetic ordering), this means violation of the Luttinger theorem which states conservation on the volume en-
closed by the Fermi surface with inclusion of interaction. The interaction is connected with the global topological excitations associated with the emergent gauge field in the system of deconfined spinons. A description of such anomalous frustrated metallic systems is provided by the fractionalized Fermi liquid (FL*) picture, which was initially formulated within the framework of the $s - d(f)$ exchange (Kondo) model. In this state, which is a kind of metallic spin liquid and has an essentially topological nature, charged excitations have conventional quantum numbers, but these coexist with additional fractionalized degrees of freedom in a second band. The FL* was applied to frustrated Kondo lattices. Also, some considerations within the Kitaev-Kondo lattice model were performed, including realization of FL* state and unconventional superconducting phases.

In the present paper we provide a modern topological description of such d- and f-compounds within the framework of the FL* picture and related theories, a comparison with simple perturbation theory being performed. We also treat the limit of strong correlations, where the picture of local moments is most physically clear. Although concepts of the FL* theory in various versions were formulated earlier, it seems to be timely to apply them to contemporary experimental situation in appropriate forms.

2. FL* state: between Fermi liquid and antiferromagnetism

RVB state can be identified with a quantum spin-liquid state — long-range entangled state possessing fractionalized excitations, which is observed in a number of frustrated systems. The theory of insulating frustrated pyrochlores was elaborated in detail in Ref. where a classification of symmetric U(1) and $Z_2$ spin liquids on the pyrochlore lattice was performed within the projective-symmetry-group framework for Fermi spinons, a comparison with the Schwinger boson approach being performed. With account of gauge fluctuations, the low temperature specific heat in the nodal-star spin liquid was calculated, the leading contribution from the bare spinons being proportional to $T^{3/2}$.

Here we focus on frustrated non-Fermi-liquid metallic systems which are subject of topological characterization, so that the FL* theory and its analogs seem to be relevant. The most important topological feature of FL* is that it possesses the small Fermi surface which does not include localized $d(f)$-electrons, unlike the usual heavy Fermi liquid (FL).

According to the Lieb-Schulz-Mattis theorem, a state with a gap and unbroken symmetry must have a ground-state degeneracy which has a topological nature. The existence of gapped spinon excitations (in the two-dimensional (2D) case) means the existence of topologically distinct sectors on a torus and protects the FL* state. The combination of the spin-liquid state and current carriers can also lead to violations of the area law for the entanglement entropy.

Usually the FL* concept is applied to 2D case, but can be generalized to 3D case owing to Oshikawa’s theorem. The FL* state was considered near both the metal-insulator transition and transition between metallic states with large and small Fermi surfaces, and includes fermionic spinon excitations which form a “ghost” Fermi surface. The corresponding phase diagrams were built in both doped case and the situation of interaction-driven transition.

In the gauge field theory, low-temperature specific heat has a singularity $C(T) \sim T \ln 1/T$ in the quantum-critical region and $U(1)$ FL* phase or $C(T) \sim T \ln 1/b_0$ in the Fermi liquid near the transition, $b_0$ being the auxiliary-boson condensate determining the mixing between local moments and conduction electrons at FL formation. Thus the specific heat coefficient $\gamma = C/T$ diverges logarithmically in the FL* phase (in the 2D case, $C(T) \sim T^{2/3}$). Besides that, $T$-linear resistivity occurs in the quantum-critical strange metal phase.

The FL* state was considered as a ground state. However, it was also concluded that this state with the spinon Fermi surface should be unstable with to a broken-symmetry AFM state, but can occur at finite temperatures. With increasing $s - d(f)$ coupling, the deconfined phase with small Fermi surface passes first into usual itinerant AFM state with a large Fermi surface volume, and then into FL state. According to a direct transition from localized AFM state to the Kondo FL state in $T = 0$ phase diagram is possible only with fine tuning via the multicritical point. Some different versions of the phase diagram were treated in detail. In particular, the approach yields a whole AFM-FL line. This situation may be viewed as an example of deconfined criticality.

Most Kondo and heavy-fermion systems demonstrate magnetic ordering and/or pronounced spin fluctuations even in the strong-coupling regime. A transition (crossover) from itinerant to localized magnetism in the Kondo lattices is to some extent analogous to the metal-insulator transition (localized moments correspond to the Hubbard subbands). Moreover, the transition to FL* phase can be treated as a partial (orbital-selective) Mott transition.

Provided that the quantum critical point and magnetic transition point coincide, the FL* theory includes two different divergent time or length scales. The first (shorter) scale describes fluctuations owing to the Fermi surface rearrangement, and the second one due to magnetic fluctuations. Thus, on the magnetically-ordered side of the quantum phase transition into the FL state, there should be an intermediate temperature regime below the coherence temperature, $T_N < T < T_{coh}$, where we have the FL* picture. Such a picture was proposed to treat properties of the frustrated layered system PdCrO$_2$. Near the metal-insulator transition, a second crossover (which is connected with condensation of spinons), and even some more crossovers, were proposed. Such crossovers can be supposed also on both above magnetic and FL phases of the Kondo lattice.

The description in terms of spinon statistics is changed from fermionic to bosonic in AFM phase after passing deconfinement transition, so that the description in terms of auxiliary particles becomes different. In particular, the Schwinger bosons are convenient to describe AFM state, and the pseudofermons to describe the Fermi-spinon picture. In this con-
The integral over $q$ in (3) is determined by the magnon spectrum. Therefore, the result (3) is valid also in the 3D frustration situation, e.g., for the 2D-like magnon spectrum

$$\omega_q^2 - q^2 \delta_x^2 + c_x^2 q_x^2 + c_y^2 q_y^2 + \cdots$$ \hfill (7)

with $c_x, c_y \ll \omega_N, \omega_F$ (another frustration model is considered in Ref. [3]). Thus at $T > T^*$ we have a marginal Fermi liquid behavior: the $T \ln T$-dependence of specific heat, and also $T \ln T$ (nearly $T$-linear) dependence of resistivity [33]. Therefore, we have an interpolation with the results of the FL$^*$ theory.

To take into account magnetic fluctuations above the FL state (at the crossover in the strong-coupling region), we can treat fluctuations of the effective $s - d(f)$ hybridization which are most important in the Kondo lattices. The standard representation of the scalar slave boson (measuring the hybridization) is insufficient to take into account spin-flip processes. Therefore we can use at finite $T$ (in the renormalized classical regime [18]) the representation (3) in terms of pseudofermions $f_i$ and bosons $b_{\nu}$,

$$b_{\nu} = \sigma^{\nu \alpha} f_i^{\dagger} e^{\alpha}_i / \sqrt{2}$$ \hfill (8)

with $\nu = 0, \ldots, 3$ and $\sigma^{\nu \alpha} = \delta^{\nu \alpha}$. The operators $b_{\nu}$ are Schwinger bosons which create local singlet and triplet states resulting from the $s - d(f)$ coupling between localized and itinerant states. In the usual picture of Kondo singlet formation, only $b_0$-boson is present, and other components describe the magnetic order fluctuations. The scattering by such fluctuations should result in a similar behavior of thermodynamic and transport properties, as described above.

To describe the exotic state with small Fermi surface in the strong-interaction case (narrow bands), the approaches by Weng (the phase string theory [35, 36] and Ribeiro-Wen [5]) were proposed. These formulations differ by statistics of auxiliary particles but seem to be on the whole equivalent. Both the approaches include subsystems of RVB states and conduction electrons, so that the wavefunction of the system can be represented as a direct product of half-filled fermionic or bosonic RVB state and conduction-electron dopon or Weng’s fermion state, respectively [37]. The approach using “backflow” fermionic spinons [54] should be also mentioned.

Consider the Hamiltonian of the $t - J$ model

$$H = \sum_{ij} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + \sum_{ij} J_{ij}(S_i \cdot S_j)$$ \hfill (9)

where

$$\tilde{c}_{i\sigma} = X_i(0, \sigma) = |0\rangle \langle i\sigma|$$ \hfill (10)

are the projected electron (Hubbard’s) operators. This model is equivalent to the narrow-band $s - d$ model [38]. The elimination of the doubly occupied states (i.e., of the upper Hubbard subband) owing to the projection just means formation of the small Fermi surface.

The dopon representation [5] for the Hubbard’s operators reads

$$\tilde{c}_{i\sigma} = -\frac{\sigma}{\sqrt{2}} \sum_{\sigma'} \tilde{d}_{i\sigma'} [S_{\sigma\sigma'} - (S_{\sigma} \cdot S_{\sigma'})].$$ \hfill (11)
where \( \sigma = \uparrow, \downarrow \) \((\pm)\), \( d_{\sigma}^{\dagger} = d_{\sigma}^{\dagger}(1 - d_{\sigma^c}^{\dagger}d_{\sigma^c}^{\dagger}) \) with \( d_{\sigma}^{\dagger} \) the Fermi dopon operators. Depending on physical picture, both Fermi spinon and Schwinger boson representations can be used for localized \( S = 1/2 \) spins \( S_i \) [5, 39]. In the Bose case, the small Fermi surface is retained, but in the Fermi case the picture can become more complicated owing to spinon-dopon hybridization. The corresponding mean-field calculations [5] enable one to describe quantitatively the spectrum of copper-oxide systems, but a more accurate treatment including gauge field fluctuations is not yet performed.

Using the many-electron Hubbard’s representation, the dopon representation is generalized to the narrow-band \( s-d \) exchange model [38] with arbitrary spin \( S \), which is appropriate for localized-moment Mn systems:

\[
H = \sum_{ij\sigma} t_{ij} g_{\sigma}^{\dagger} g_{\sigma} + \sum_{ij} J_{ij}(S_i \cdot S_j),
\]

where

\[
g_{\sigma}^{\dagger} = \sum_{\sigma'} c_{\sigma'}^{\dagger}(1 - n_{i,-\sigma'}) S_{\delta_{\sigma\sigma'}} - (S \cdot \sigma_{\sigma'}) / 2S + 1.
\]

The result [13] corresponds to the double-exchange theory by Kubo and Ohata [40], which is also appropriate for manganites.

Thus in the cases of both strong and weak \( s-d(f) \) interactions we have a description in terms of the two-band picture within different models.

3. Discussion and conclusions

Now we discuss frustration effects in real metallic systems. A number of Kondo and heavy-fermion compounds demonstrate frustrated magnetism and non-Fermi-liquid behavior (see, e.g., [8]). In the distorted kagome system CePdAl magnetic frustration of 4f-moments results in a paramagnetic quantum-critical phase with non-Fermi-liquid behavior of resistivity [41, 42]. This picture includes also a Mott-type f-electron partial delocalization (transition from small to large Fermi surface) [42]. Two-dimensional fluctuations at the quantum-critical point are observed in CePdAl [41], CeCu6–xAu x [43] and YbRh2Si2 [44].

The electronic state of \( Y_2Ir_2O_7 \) pyrochlores is insulating. In the hole-doped \( Y_{2-x}Cu_xCaIr_2O_7 \) system, the resistivity becomes much smaller than that of pure compound and has a metallic \( T \)-linear behavior with a small upturn below around 15 K. According to \( \mu \)SR measurements, the AFM long-range ordered state occurs in pure case, while the ground state of the doped system is non-magnetic up to 2 K [45]. Thus the antiferromagnetism is suppressed by doping, the system being changed from insulator to metal. From these results, the authors propose that there is a quantum critical point governed by doping. This picture is similar to the phase diagram of copper-oxide systems [3].

It is important that, upon doping, \( Z_2 \) spin liquid can pass to superconducting state owing to spinon pairing [18], as it is discussed in the case of cuprates in Ref. [3]. Indeed, superconductivity with rather high \( T_c \) is observed in the metallic pyrochlores \( KOs_2O_6 \) (\( T_c = 9.6 \) K [46]), \( RhO_2S_2O_6 \) (\( T_c = 6.4 \) K [47], \( \gamma = 34 \) mJ/mol·K²), and \( CsOs_2O_6 \) (\( T_c = 3.3 \) K [48]).

In pure \( \beta-Mn \), \( \gamma = 80 \) mJ/mol·K² [14] and NFL behavior is observed [15]; \( \gamma \) decreases upon doping with occurrence of AFM ordering and increasing the Neel temperature [49].

According to Ref. [50], the magnetism of \( \beta-Mn \) can be reduced to that of an infinite network of corner-sharing triangles, which is in some respects identical to the 2D kagome lattice; besides that, \( \beta-Mn \) is not a “weak” magnet, but a rather strong magnet with a large dynamical moment up to lowest \( T \). Basing on polarized-neutron scattering experiments, the authors of Ref. [51] demonstrate the presence of emergent spin structures resembling the triangular-lattice antiferromagnet and collective states within networks in Co-doped \( \beta-Mn \).

According to Ref. [52], in the \( Mn_2FeAl \) compound with the \( \beta-Mn \) structure, frustrated antiferromagnetism coexists with large \( \gamma = 210 \) mJ/mol·K².

The compound \( YMn_2 \) has a lattice structure similar to pyrochlores and a frustrated AFM structure, demonstrating strong short-range order above \( T_N \). In the doped system \( Y_{1-x}Se_xMn_2 \) with \( x \) = 0.03 or under pressure, the long-range order is destroyed, while \( \gamma \) reaches very large value, 140 mJ/mol·K² [16].

Inelastic neutron scattering measurements on a single crystal of \( Y_{1-x}Se_xMn_2 \) demonstrate that the dynamical susceptibility indicates a degeneracy of magnetic states. Moreover, spins seem to be correlated and form short-lived four-site collective spin singlets. Such a frustrated heavy-fermion behavior is quite unusual within the picture of itinerant magnetism [53].

To conclude, the topological treatment within the two-band model clarifies the physical picture and enables one to unify frustrations, Kondo and spin-fluctuation (e.g., electron-magnon) mechanisms which were considered earlier separately [12, 13]. A comparison with perturbation theory and strong correlation limit permits to obtain a consistent picture of peculiar magnetic, thermodynamic and transport properties of \( d \)- and \( f \)-compounds, especially anomalies of specific heat.

The topological picture is supported by formation of the small Fermi surface in magnetically frustrated systems (contrary to usual Kondo lattices). More generally, these arguments can be related to the problem of Hubbard subbands [54] and disordered local moments which violate the Fermi liquid picture and Luttinger theorem too [55]. To treat these questions in more detail, a consistent consideration of gauge field effects with proper account of constraints would be instructive. The involved problem of describing spinon statistics is also far from final solution.

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