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Hubbard Bands and Exotic States in Doped and Undoped Mott Systems: The Kotliar–Ruckenstein Representation

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Abstract: The slave–particle representation is a promising method to treat the properties of exotic strongly correlated systems. We develop a unified approach to describe both the paramagnetic state with possible spin–liquid features and states with strong long-range or short-range magnetic order. Combining the Kotliar–Ruckenstein representation and fractionalized spin–liquid deconfinement picture, the Mott transition and Hubbard subbands are considered. The spectrum in the insulating state is significantly affected by the presence of the spinon spin–liquid spectrum and a hidden Fermi surface. Presenting a modification of the Kotliar–Ruckenstein representation in the spin–wave region, we treat the case of magnetic order, with special attention being paid to the half-metallic ferromagnetic state. The formation of small and large Fermi surfaces for doped current carriers in the antiferromagnetic state is also discussed.

Keywords: Mott insulators; Hubbard model; slave–particle representations; spin liquids; magnetism



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1. Introduction

The problem of describing strongly correlated states has been a topic of interest and significance for a long time. In particular, here belong the aspects of the Mott transition, which refers to the correlation-driven transition from a metallic state to an insulating state [1]. The related physical phenomena occur in a number of doped and undoped Mott systems, including insulators and metals with exotic properties [2].

The physics of Mott systems originates from the competition of magnetism, Coulomb correlations, frustration, and topology. Typically (in most d-metal compounds), the Mott transition occurs according to the Slater mechanism, i.e., involves the insulating phase with antiferromagnetic band splitting (see, e.g., ref. [3]). However, the situation changes when dealing with frustrated systems that do not demonstrate antiferromagnetic ordering, so that only the paramagnetic metallic and insulator states (possibly, with unusual characteristics) are present, leading to the formation of a spin–liquid-type state [4,5].

Such a transition into the insulator state, known as the Mott scenario, is associated with the correlation Hubbard splitting. In the Mott state, the spectrum exhibits a significant charge gap that is determined by bosonic excitation branches. Consequently, the electrons become composite particles and undergo fractionalization, where the spin characteristics are controlled by neutral fermions called spinons, and the charge ones by bosons [6,7]. This concept can be formalized by using the slave–boson representations [6–8].

The interaction between bosons and fermions mediated by a gauge field plays a significant role as it gives rise to confinement [7]. This leads to a transition toward a confinement metallic state, which is marked by the occurrence of Bose condensation and a non-zero residue in the electron Green’s function. Conversely, in the insulator state, the bosons have a gap in their energy spectrum, leading to an incoherent overall spectrum that encompasses Hubbard’s bands. In this case, the electron Green’s function is a combination of the boson and fermion Green’s functions through convolution.

Recent theoretical advancements have offered a fresh perspective on the Mott transition by introducing a topological framework. This is particularly relevant because spin

liquids, known for their topological order, are involved in this transition. In the study of phase transitions in magnetically frustrated systems, the consideration of topological excitations becomes essential as they play a significant role in confinement. These ideas have been extensively reviewed, e.g., in refs. [9,10].

As for doped Mott systems, copper-oxide materials which are basic for high- T_c superconductors should be mentioned in the first place. In the overdoped case, the normal (non-superconducting) ground state is characterized as a Fermi liquid with a “large” Fermi surface (including both localized and itinerant states), where Luttinger’s theorem holds. At the same time, in the underdoped case, the ground state is more complicated and may possess small hole pockets of the Fermi surface [7,11]. The description of this state depends again on the presence or absence of antiferromagnetic ordering. The small Fermi surface can occur not only in the case of long-range order but also in the situation of strong short-range order [12–14].

In this paper, we examine the metal-insulator transition through a topological perspective, specifically focusing on spin-charge separation within the framework of the Kotliar–Ruckenstein slave-boson representation. We employ the deconfinement concept to investigate the Hubbard subbands’ spectrum. Our treatment aims to understand the Mott transition leading to a spin-liquid state, while also establishing the connection between the charge gap in the boson spectrum and the Hubbard splitting.

The idea of preserving the Fermi surface during a quantum phase transition is supported by the presence of a spinon Fermi surface in the paramagnetic phase of a Mott insulator [5]. In a gapped phase like the Mott state, the traditional Fermi surface does not exist and instead transforms into a hidden or ghost Fermi surface. However, the volume enclosed by the Fermi surface, as described by the Luttinger theorem, remains conserved [15]. This concept has also been applied to half-metallic ferromagnets [16,17]. In this study, we expand upon this approach and demonstrate how to combine the concept of composite particles with spin-liquid states and magnetic ordering in various cases.

In Section 2, we review various versions of the slave-boson representations. In Section 3, we treat the problem of metal-insulator in the paramagnetic case. Although we apply the standard Kotliar–Ruckenstein representation used in previous works [18,19], we provide a new interpretation which takes into account spin-charge separation in terms of exotic quasiparticles—spinons and holons. In Section 4, we derive a new form of the Kotliar–Ruckenstein representation, which is compatible with the approach of many-electron Hubbard operators [20] and is convenient in the magnetic state. We apply this form to treat conducting ferromagnets and antiferromagnets. In Section 5, a discussion is presented.

2. Slave-Particle Representations of the Hubbard Model

The Hamiltonian of the Hubbard model reads

$$\mathcal{H} = - \sum_{ij\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + \mathcal{H}_d, \quad (1)$$

where $c_{i\sigma}^\dagger$ are electron creation operators. The Heisenberg interaction

$$H_d = \sum_{ij} J_{ij} \mathbf{S}_i \mathbf{S}_j, \quad (2)$$

which can arise as an effective superexchange interaction in the second order of perturbation theory in the Hubbard model, is explicitly incorporated for further ease of representation. Such a mixed representation is known as $t - J - U$ model, which reduces in the large- U limit to the well-known $t - J$ model (see, e.g., the review [21]). The Hamiltonian of the latter model for hole doping can be represented in the form

$$\mathcal{H} = \sum_{ij\sigma} t_{ij} \tilde{c}_{i\sigma}^\dagger \tilde{c}_{j\sigma} + \mathcal{H}_d \quad (3)$$

where $\tilde{c}_{i\sigma}^\dagger = X_i(0\sigma) = |i0\rangle\langle i\sigma| = c_{i\sigma}(1 - n_{i-\sigma})$ are the Hubbard projection operators creating empty on-site states.

In situations where strong correlation effects are dominant, it is often useful to employ auxiliary or “slave” boson and fermion representations. The slave–boson representation was proposed in the pioneering works by Barnes [22] and Coleman [23] for the Anderson models and developed by many authors.

Anderson [6] proposed a physical interpretation of the slave–boson representation for the Hubbard model based on the concept of separating the spin and charge degrees of freedom of an electron,

$$c_{i\sigma} = X_i(0, \sigma) + \sigma X_i(-\sigma, 2) = e_i^\dagger f_{i\sigma} + \sigma d_i f_{i-\sigma}^\dagger. \quad (4)$$

where $\sigma = \pm 1$, $f_{i\sigma}$ are the annihilation operators for neutral fermions (spinons), and e_i , d_i for charged spinless bosons (holons and doublons). In the large- U limit, we have to retain in (4) only the first (second) term for the hole (electron) doping.

Alternatively, the slave–fermion representation which uses the Schwinger boson operators $b_{i\sigma}$ can be used (see, e.g., ref. [24]),

$$X_i(0, \sigma) = f_i^\dagger b_{i\sigma}, \quad X_i(+, -) = b_{i\uparrow}^\dagger b_{i\downarrow}, \quad (5)$$

so that

$$\sum_{\sigma} b_{i\sigma}^\dagger b_{i\sigma} + f_i^\dagger f_i = 1. \quad (6)$$

This representation is more suitable in the case of magnetic ordering. Such uncertainty in the statistics of excitations leads to difficulties in constructing a unified picture and requires more advanced approaches.

A more complicated representation was proposed by Kotliar and Ruckenstein [8]. This uses the Bose operators e_i , $p_{i\sigma}$, d_i and Fermi operators $f_{i\sigma}$:

$$c_{i\sigma}^\dagger \rightarrow f_{i\sigma}^\dagger z_{i\sigma}^\dagger, \quad z_{i\sigma}^\dagger = g_{2i\sigma} (p_{i\sigma}^\dagger e_i + d_i^\dagger p_{i-\sigma}) g_{1i\sigma}, \quad (7)$$

with the constraints

$$\sum_{\sigma} p_{i\sigma}^\dagger p_{i\sigma} + e_i^\dagger e_i + d_i^\dagger d_i = 1, \quad f_{i\sigma}^\dagger f_{i\sigma} = p_{i\sigma}^\dagger p_{i\sigma} + d_i^\dagger d_i, \quad (8)$$

which can be used to introduce gauge fields [7].

According to Kotliar and Ruckenstein, the representation of many-electron operators is not fixed and can include additional operator factors as long as they have eigenvalues of 1 in the physical subspace. While all these forms yield accurate results in exact treatments, they may differ in approximate calculations. This is particularly significant when constructing mean-field approximations as it allows for agreement with limiting cases. Thus, the factors $g_{1,2i\sigma}$ are somewhat arbitrary, but to obtain an agreement with the Hartree–Fock limit, one uses the values

$$g_{1i\sigma} = (1 - d_i^\dagger d_i - p_{i\sigma}^\dagger p_{i\sigma})^{-1/2}, \\ g_{2i\sigma} = (1 - e_i^\dagger e_i - p_{i-\sigma}^\dagger p_{i-\sigma})^{-1/2}. \quad (9)$$

In the mean-field approximation for a non-doped case and a non-magnetic state, we can put $g_{1,2\sigma}^2 = 2$. It should be noted that such a choice results in some difficulties, in particular leading to inconsistency in the atomic limit [19]. Also, we will see below that this choice is inadequate in a magnetic state.

In the framework of various slave–boson approaches, a number of mean-field theories were developed [7]. In particular, treatments within the Kotliar and Ruckenstein representations on saddle-point level became popular because of their good agreement with numerical simulations. However, such treatments are not free of difficulties [25,26]. Generally speaking, they suffer from drawbacks connected with spurious Bose conden-

sation. To overcome this difficulty and develop more advanced theories, one can use the $1/N$ -expansion [23] or gauge-field theories which are extensively discussed in the review [7]. In this connection, treatments of the limiting cases, where the slave-boson approach is exact or controlled [27,28], can be useful.

To take into account spin-flip processes, it is suitable to use the rotationally invariant version [29,30]. Here, the projected electron is represented as a composite of Fermi spinon with scalar and vector bosons p_{i0} and \mathbf{p}_i . Using the coupling rule of momenta 1 and $1/2$ one obtains

$$c_{i\sigma} = \sum_{\sigma'} (e_i^\dagger p_{i\sigma'\sigma} + \sigma p_{i-\sigma-\sigma'}^\dagger d_i) f_{i\sigma'} \quad (10)$$

with

$$\hat{p}_i = \frac{1}{2}(p_{i0}\sigma_0 + \mathbf{p}_i\sigma) \quad (11)$$

and the constraints

$$e_i^\dagger e_i + \sum_{\mu=0}^3 p_{i\mu}^\dagger p_{i\mu} + d_i^\dagger d_i = 1, \quad (12)$$

$$\sum_{\sigma} f_{i\sigma}^\dagger f_{i\sigma} = \sum_{\mu=0}^3 p_{i\mu}^\dagger p_{i\mu} + 2d_i^\dagger d_i. \quad (13)$$

Introducing proper factors one has [30]

$$c_{i\sigma} = \sum_{\sigma'} f_{i\sigma'} z_{i\sigma'\sigma}, \quad \hat{z}_i = e_i^\dagger \hat{L}_i M_i \hat{R}_i \hat{p}_i + \hat{\tilde{p}}_i^\dagger \hat{L}_i M_i \hat{R}_i d_i \quad (14)$$

where

$$\hat{L}_i = [(1 - d_i^\dagger d_i)\sigma_0 - 2\hat{p}_i^\dagger \hat{p}_i]^{-1/2} \quad (15)$$

$$\hat{R}_i = [(1 - e_i^\dagger e_i)\sigma_0 - 2\hat{\tilde{p}}_i^\dagger \hat{\tilde{p}}_i]^{-1/2} \quad (16)$$

$$M_i = (1 + e_i^\dagger e_i + \sum_{\mu=0}^3 p_{i\mu}^\dagger p_{i\mu} + d_i^\dagger d_i)^{1/2}. \quad (17)$$

The additional square-root factors in (15)–(17) can be treated in the spirit of mean-field approximation. In particular, the factor M is equal to $\sqrt{2}$ due to the sum rule (12) and enables one to obtain an agreement with the small- U limit and with the saturated ferromagnetic case. The scalar and vector bosons p_{i0} and \mathbf{p}_i are introduced as

$$\hat{p}_i = \frac{1}{2}(p_{i0}\sigma_0 + \mathbf{p}_i\sigma) \quad (18)$$

with σ being Pauli matrices and $\hat{\tilde{p}}_i = (1/2)(p_{i0}\sigma_0 - \mathbf{p}_i\sigma)$ the time reverse of operator \hat{p}_i .

In Section 4, we will extensively employ the rotationally invariant representation to treat in detail the magnetically ordered case. We will perform the corresponding analytical transformations and demonstrate that the full form of the radicals plays an important role. In particular, this is crucial to describe incoherent states in a ferromagnet.

3. Mott Transition and Hubbard Bands in the Paramagnetic and Spin-Liquid State

In order to treat the Mott transition in frustrated systems within the paramagnetic phase, several studies [5,31,32] utilized the rotor representation. While this representation is straightforward, it is not ideal as it does not explicitly incorporate the spectrum of both Hubbard bands. An alternative description of the Mott transition and Hubbard bands can be obtained within the Kotliar–Ruckenstein representation [18,19]. These works use a Gutzwiller-type approach for a structureless paramagnetic state. Here, we perform a more advanced treatment with an account of the possible spin-liquid picture. To take into

account spin frustrations, we include explicitly the model of the Heisenberg interaction. Then, the Lagrangian of the Hubbard–Heisenberg model has the form

$$\begin{aligned}\mathcal{L} = & -\sum_{ij\sigma} t_{ij} z_{i\sigma}^{\dagger} z_{j\sigma} f_{i\sigma}^{\dagger} f_{j\sigma} + \sum_{i\sigma} f_{i\sigma}^{\dagger} (\partial_{\tau} - \mu + \lambda_{2\sigma}) f_{i\sigma} \\ & + \sum_{i\sigma} p_{i\sigma}^{\dagger} (\partial_{\tau} + \lambda_1 - \lambda_{2\sigma}) p_{i\sigma} + \sum_i e_i^{\dagger} (\partial_{\tau} + \lambda_1) e_i \\ & + \sum_i d_i^{\dagger} (\partial_{\tau} + \lambda_1 - \sum_{\sigma} \lambda_{2\sigma} + U) d_i + \mathcal{H}_d.\end{aligned}\quad (19)$$

By employing the Heisenberg Hamiltonian in the f -pseudofermion representation, it is possible to analyze spin degrees of freedom independently. In certain circumstances, it is anticipated that a spin-liquid state may emerge, characterized by excitations primarily consisting of spinons, which are neutral fermions.

In the mean-field approximation, the Lagrange factors $\lambda_{1,2}$ associated with (8) are not dependent on the specific sites. When in the insulator phase, it has been established by Lavagna [18] that $\lambda_1 = \lambda_{2\sigma} = U(1 \pm \zeta)/2$ equals the chemical potential for an infinitesimally small electron or hole doping (the addition or removal of an electron), $\zeta = (1 - 1/u)^{1/2}$, $u = U/U_c$. Here,

$$U_c = 4p^2 g_1^2 g_2^2 \varepsilon = 8\varepsilon$$

is the critical value for the Mott transition in the Brinkman–Rice approximation (see ref. [33]), $\varepsilon = 2 \left| \int_{-\infty}^{\mu} d\omega \omega \rho(\omega) \right|$ the average energy of non-interacting electron system, $\rho(\omega)$ the bare density of states.

Following refs. [18,33], we introduce the variable $x = e + d$. Then, we obtain for $y = 1/x^2$, the cubic equation

$$y^3 - (u - 1)y/u\delta^2 = 1/u\delta^2. \quad (20)$$

Earlier, the solution of this equation was discussed in refs. [18,30]. Here, we present the solution in a more convenient form. Passing to the variable $1/y$ and using a trigonometric solution of the cubic equation we derive for $u < 1$ (correlated metal phase)

$$y = 2 \left(\frac{1-u}{3u\delta^2} \right)^{1/2} \sinh \left(\frac{1}{3} \operatorname{arcsinh} \frac{\delta}{\delta_0} \right) \quad (21)$$

For $u > 1$ one has

$$y = 2 \left(\frac{u-1}{3u\delta^2} \right)^{1/2} \times \begin{cases} \cos \left(\frac{1}{3} \arccos(\delta/\delta_0) \right), & \delta < \delta_0 \\ \cosh \left(\frac{1}{3} \operatorname{arccosh}(\delta/\delta_0) \right), & \delta > \delta_0 \end{cases} \quad (22)$$

where

$$\delta_0 = 2|u-1|^{3/2}/(27u)^{1/2} \quad (23)$$

This solution is a smooth and analytic function of doping δ in the whole region $\delta < 1$. For small $\delta \ll \delta_0$ we have

$$x^2 = 1/y = \begin{cases} 1-u + O(\delta^2), & u < 1 \\ \delta/\sqrt{1-1/u}, & u > 1 \end{cases} \quad (24)$$

Generally, a considerable U -dependence takes place at any δ . For $\delta \gg \delta_0$ (close to the Mott transition) we have $x^2 \simeq \delta^{2/3}$.

The behavior (24) can be considerably changed when taking into account gauge fluctuations [5,34], especially in the two-dimensional case where intermediate energy and temperature scales can occur beyond the mean-field picture.

It is convenient to introduce the boson combination $b_i^{\dagger} = e_i^{\dagger} + d_i$ yields (cf. Ref. [19]). The expression of the corresponding Green's function takes the form

$$D(\mathbf{q}, \omega) = \langle \langle b_{\mathbf{q}} | b_{\mathbf{q}}^{\dagger} \rangle \rangle_{\omega} = \sum_{a=1,2} \frac{Z_{a\mathbf{q}}}{\omega - \omega_{a\mathbf{q}}}, \quad (25)$$

$$Z_{a\mathbf{q}} = (-1)^a U / \sqrt{U^2 \zeta^2 + U(U_c - 4\Sigma(\mathbf{q}))} \quad (26)$$

with the spectrum of boson subsystem

$$\omega_{a\mathbf{q}} = \frac{1}{2} [\pm U \zeta - (-1)^a \sqrt{U^2 \zeta^2 + U(U_c - 4\Sigma(\mathbf{q}))}] \quad (27)$$

One of two boson branches becomes gapless and provides the formation of the boson condensate at the Mott transition.

To obtain the boson self-energy, we perform a decoupling of the first term in (19), which yields essentially the correlation correction first introduced in ref. [35]. The result reads

$$\Sigma(\mathbf{q}) = -p^2 g_1^2 g_2^2 \sum_{\mathbf{k}\sigma} t_{\mathbf{k}-\mathbf{q}} n_{\mathbf{k}\sigma}, \quad n_{\mathbf{k}\sigma} = \langle f_{\mathbf{k}\sigma}^{\dagger} f_{\mathbf{k}\sigma} \rangle. \quad (28)$$

In ref. [19], the limit of vanishing renormalized electron bandwidth (i.e., bearing in mind the Mott phase where the averages $e, d \rightarrow 0$) was treated in a Gutzwiller-type approach. Here, we use a more straightforward approach: a finite bandwidth of holons occurs in a natural way by taking into account the spinon dispersion. Note that earlier, a similar consideration was performed for the $t - J$ model [7].

The presence of a small (as compared to electron energies) characteristic scale of spinon energies is crucial. As a result, the temperature dependence of the spinon Fermi surface becomes significant. This scenario shares similarities with the situation observed in magnetic order (e.g., band splitting owing to long- or short-range antiferromagnetic ordering). The dispersion of bosons is affected by the specific characteristics of the fermion spectrum, which are determined by the state of the f -system.

The spinon spectrum $E_{\mathbf{k}}$ can be stabilized in the mean-field scenario through either a non-compact gauge field or by having gapless Fermi excitations [5,36,37]. In the insulator state, this spectrum remains unaffected by bosons, leading to the emergence of various spin-liquid phases [7].

When there is minimal dependence on \mathbf{k} of $n_{\mathbf{k}\sigma}$ (indicating a localized spin phase without fermion hopping), the value of Σ approaches zero. However, in the case of a spin liquid, a distinct Fermi surface is present. Despite the spectrum of spinons can differ from that of bare electrons; putting $q = 0$, we still obtain $\Sigma(0) = U_c/4$ since the spinon band is half-filled and the position of the Fermi energy (the chemical potential) remains fixed.

In the nearest-neighbor approximation, when converting Equation (28) into real-space representation, it becomes evident that the spinon spectrum and the correction to the holon spectrum vary only in terms of replacing the parameter J with t ($\Sigma(\mathbf{q}) \propto E(\mathbf{q})$, as described in ref. [7] for the $t - J$ model). Specifically, we can observe that

$$\begin{aligned} \Sigma(\mathbf{q}) &= U_c (\cos q_x + \cos q_y) / 8, \\ \Sigma(\mathbf{q}) &= \pm U_c \sqrt{\cos^2 q_x + \cos^2 q_y} / (4\sqrt{2}) \end{aligned} \quad (29)$$

for Anderson's uniform resonating valence bond (uRVB) and π -flux (π FI) phases, respectively. Thus, in the case of the uRVB state, the quasimomentum dependences of electron and spinon spectrum coincide: $E_{\mathbf{k}} \sim J(\cos k_x + \cos k_y)$. At the same time, our method enables one to treat a more general situation. So, in the π FI phase (which includes Dirac points) $E_{\mathbf{k}} \sim \pm J \sqrt{\cos^2 k_x + \cos^2 k_y}$. For the gapped Z_2 phase, which can occur in the presence of next-nearest-neighbor interactions, the mapping of the spectra is violated and the consideration is more difficult.

In the case of large U , we have two well-separated bands

$$\omega_{a\mathbf{q}} = \text{const} - (-1)^a \Sigma(\mathbf{q}) / \zeta.$$

The observable electron Green's function is obtained as a convolution of the boson and spinon Green's functions [7,19,37]. For $J \ll |t|$, this spinon smearing does not strongly influence the shape or density of the state. Then, we can put $\text{Im}\langle\langle f_{\mathbf{k}\alpha} | f_{\mathbf{k}\alpha}^\dagger \rangle\rangle_E \sim \delta(E - \lambda_2)$ to obtain the Hubbard bands with the energies $\lambda_2 - \omega_{1,2\mathbf{q}}$ for vanishing electron (hole) doping with energies near 0 and U , respectively, λ_2 being the corresponding chemical potential [19]. This energy spectrum consists of upper and lower Hubbard subbands, each with a width of the order of the bare bandwidth. At the transition point, where the interaction strength approaches the critical value U_c , the energy gap between these subbands diminishes and eventually closes. A further analysis of collective modes arising from the Hubbard bands with account of doping was performed in ref. [38].

4. Magnetic States of the Doped Mott Insulator

4.1. Derivation of the Hamiltonian in the Spin-Wave Region

For magnetically ordered phases with strong long-range or short-range order, the approximations of the previous section do not work since the above approximation for factors g is not valid [16]. Most simple is the case of ferromagnetic ordering, which was investigated earlier in terms of Hubbard's operators [39,40]. According to Nagaoka [41], the ground state in the large- U limit is a saturated ferromagnet for one excess hole (or double); this conclusion can be extended in the case of finite doping, as demonstrated from analysis of instabilities of this state, which can be characterized as a half-metallic ferromagnet with an energy gap for one of the spin projections [39,40].

The original version of the Kotliar–Ruckenstein representation (7) provides a mean-field description, but turns out to be insufficient since it does not describe spin-flip processes, which are crucial to describing incoherent states. Therefore, we use the rotationally invariant representation (10) and carry out its further transformations.

The square-root factors in (17) can be treated in the spirit of the mean-field approximation. Correspondingly, the factor M is $\sqrt{2}$ due to the sum rule (12); this permits us to obtain an agreement with the free-electron limit and with the ferromagnetic case.

According to ref. [30], we have

$$\mathbf{S} = \frac{1}{2} \sum_{\sigma\sigma'} \sigma_{\sigma\sigma'} p_{\sigma\sigma_1}^\dagger p_{\sigma_2\sigma'} = \frac{1}{2} (p_0^\dagger \bar{\mathbf{p}} + \bar{\mathbf{p}}^\dagger p_0 - i[\bar{\mathbf{p}}^\dagger \times \bar{\mathbf{p}}]) \quad (30)$$

with $\bar{\mathbf{p}} = (p^x, -p^y, p^z)$. Then, we derive

$$\begin{aligned} S^z &= \frac{1}{2} (p_0^\dagger p_z + p_z^\dagger p_0 + i(p_x^\dagger p_y - p_y^\dagger p_x)) \\ &= \frac{1}{2} (p_0^\dagger p_z + p_z^\dagger p_0 + p^{++} p^+ - p^{--} p^-) \end{aligned} \quad (31)$$

$$\begin{aligned} S^+ &= \frac{1}{\sqrt{2}} ((p_0^\dagger + p_z^\dagger) p^- + p^{++} (p_0 - p_z)) \end{aligned} \quad (32)$$

where $p^\pm = (p_x \pm ip_y)/\sqrt{2}$ and we have taken into account (12). One can see that commutation relations for spin operators are exactly satisfied, unlike the linearized Holstein–Primakoff representation.

For a Heisenberg ferromagnet ($p_0 \simeq p^z \simeq 2^{-1/2}$), we obtain $S_i^+ \simeq p_i^-$ to lowest-order approximation, so that the Heisenberg Hamiltonian takes the usual spin-wave form

$$\mathcal{H}_d = \sum_{\mathbf{q}} \omega_{\mathbf{q}} p_{\mathbf{q}}^{-\dagger} p_{\mathbf{q}}^- + \text{const}, \quad \omega_{\mathbf{q}} = J_{\mathbf{q}} - J_0 \quad (33)$$

It is crucial to highlight that in order to achieve this outcome, it is essential to retain the vector product in Equation (30) to prevent the mixing of the bosons p and p^\dagger . This

retainment differs from the approach employed in ref. [30] for the paramagnetic phase. Note that in the magnetic ordering case, p_i^+ is not related to spin operators, see (31) and (32).

Equation (14) can be simplified in the case of half-metallic ferromagnetism near half-filling (small doping, band filling $n \lesssim 1$) where, in the mean-field approach, $p_0 = p_z = p \simeq 1/\sqrt{2}$, $e \simeq \langle e \rangle = (1 - n)^{1/2}$. Taking into account the relation

$$2\hat{p}_i^\dagger \hat{p}_i = \frac{1}{2}(p_{i0}^2 \sigma_0 + (\mathbf{S}_i \sigma)) \quad (34)$$

we obtain

$$L = \begin{pmatrix} 1 - p_0^2 - S^z & -S^+ \\ -S^- & 1 - p_0^2 + S^z \end{pmatrix}^{-1/2}, \quad (35)$$

$$R = \begin{pmatrix} 1 - p_0^2 + S^z - e_i^\dagger e_i & -S^- \\ -S^+ & 1 - p_0^2 - S^z - e_i^\dagger e_i \end{pmatrix}^{-1/2}, \quad (36)$$

$$p = \begin{pmatrix} p_0 + p_z & p^- \\ p^+ & p_0 - p_z \end{pmatrix} \quad (37)$$

Using the sum rule (12) and retaining only diagonal terms we obtain $L_{++} \sim 1/|e|$, $R_{--} \sim 1/|p^\pm|$. Neglecting the terms proportional to holon operators we derive in the large- U limit. Thus, the factor e^\dagger in the numerator of (14) is canceled and we derive in the large- U limit for the projected operator of hole creation

$$\tilde{c}_{i\sigma}^\dagger = \sqrt{2} \sum_{\sigma'} \hat{p}_{i\sigma\sigma'} f_{i\sigma} = \frac{1}{\sqrt{2}} \sum_{\sigma'} f_{i\sigma'} [\delta_{\sigma\sigma'} p_{i0} + (\mathbf{p}_i \sigma_{\sigma'\sigma})] \quad (38)$$

or

$$\begin{aligned} \tilde{c}_{i\uparrow}^\dagger &= \frac{1}{\sqrt{2}} f_{i\uparrow} (p_{i0} + p_{iz}) + f_{i\downarrow} p_i^+ \\ \tilde{c}_{i\downarrow}^\dagger &= \frac{1}{\sqrt{2}} f_{i\downarrow} (p_{i0} - p_{iz}) + f_{i\uparrow} p_i^-. \end{aligned} \quad (39)$$

In particular, this representation satisfies the exact commutation relations for Hubbard's operators. However, the multiplication rule, which is crucial for calculations,

$$X_i(0, -) = X_i(0, +) X_i(+, -) \quad (40)$$

is satisfied only approximately ($\frac{1}{\sqrt{2}}(p_{i0} + p_{iz}) \simeq 1$, $X_i(+, -) \simeq p_i^-$).

In the derivation of (39), which was first performed in ref. [16], the spin-wave correction in matrices L and R was neglected to replace the operator S^z by $1/2$. We can make the next step by noting that according to (31), (32), and (8)

$$\sqrt{1/2 \pm S^z} \simeq \sqrt{1/2 \pm 2p_0 p_z / 2} \simeq (p_0 \pm p_z) / \sqrt{2} \quad (41)$$

(a more strict derivation may be performed within the path integral approach). Then, we can write the representation in terms of spin operators,

$$\tilde{c}_{i\sigma} = \sum_{\sigma'} f_{i\sigma'}^\dagger \left[\frac{1}{2} \delta_{\sigma\sigma'} + (\mathbf{S}_i \sigma_{\sigma'\sigma}) \right] \quad (42)$$

or

$$\begin{aligned} \tilde{c}_{i\uparrow} &= f_{i\uparrow}^\dagger \left(\frac{1}{2} + S_i^z \right) + f_{i\downarrow}^\dagger S_i^+ \\ \tilde{c}_{i\downarrow} &= f_{i\downarrow}^\dagger \left(\frac{1}{2} - S_i^z \right) + f_{i\uparrow}^\dagger S_i^-. \end{aligned} \quad (43)$$

Although it was justified above for small doping and magnetic states only, it seems to be reasonable in a more general situation, as will be discussed below.

4.2. Electron States and Spin Waves in the Strongly Correlated Hubbard Model

Now we can consider the electron and spin Green's functions for a saturated ferromagnet with the use of the Hamiltonian (3). In such a situation of small hole doping, the spin-up spinon states propagate freely and their band is almost half-filled, so that

$$\tilde{n}_{\mathbf{k}} = \langle f_{\mathbf{k}\uparrow} f_{\mathbf{k}\uparrow}^\dagger \rangle = n(t_{\mathbf{k}})$$

with $n(E)$ being the Fermi function.

The representation (43) retains commutation relations for Hubbard's X-operators and even the multiplication rule (40), so that the calculations of electron and spin-wave spectra can be performed step-by-step in analogy with [39,40] with expansion in occupation numbers of holes and magnons.

Although the correlated electrons (holes), described by the operators (39) and (43), are composite particles, the spin-up states propagate freely on the background of the ferromagnetic ordering, the temperature correction being proportional to $T^{5/2}$ owing to rotational invariance (however, the residue of the electron Green's function has a more strong $T^{3/2}$ dependence). Physically, this free motion is due to condensation of p_z -bosons.

On the other hand, the situation is quite non-trivial for spin-down states. Such a state is a complex of spinon f_{\uparrow}^\dagger and boson $(p^-)^\dagger$ so that in the simplest approximation, we can write down the convolution of the spinon and magnon Green's functions to obtain

$$G_{\mathbf{k}\downarrow}^0(E) = \sum_{\mathbf{q}} \frac{\tilde{n}_{\mathbf{k}+\mathbf{q}} + N(\omega_{\mathbf{q}})}{E - t_{\mathbf{k}+\mathbf{q}} + \omega_{\mathbf{q}}} \quad (44)$$

with $N(\omega)$ the Bose function. It should be noted that this result can be also reproduced starting from the boson representation (39), ref. [16] and even in the more simple Schwinger boson representation (5), see ref. [17]. The instability of the saturated (half-metallic) state is described as the condensation of these bosons.

To improve the approximation and describe the instability, we write down the equation of motion for Green's function

$$G_{\mathbf{k}\downarrow}(E) = \langle \langle \tilde{c}_{\mathbf{k}\downarrow} | \tilde{c}_{\mathbf{k}\downarrow}^\dagger \rangle \rangle_E = \sum_{\mathbf{q}} \Gamma_{\mathbf{k}\mathbf{q}}(E), \quad (45)$$

$$\Gamma_{\mathbf{k}\mathbf{q}}(E) = \sum_{\mathbf{q}'} \langle \langle S_{\mathbf{q}}^- f_{\mathbf{q}-\mathbf{k}\uparrow}^\dagger | f_{\mathbf{q}'-\mathbf{k}\uparrow} S_{-\mathbf{q}'}^+ \rangle \rangle_E \quad (46)$$

(note that the terms with f_{\downarrow} do not work in low orders). Commuting the operator $S_{\mathbf{q}}^-$ with the Hamiltonian (3) and performing decoupling we obtain for $T = 0$ the equation for the Green's function in the right-hand side of (46)

$$\begin{aligned} (E - t_{\mathbf{k}-\mathbf{q}} + \omega_{\mathbf{q}}) \Gamma_{\mathbf{k}\mathbf{q}}(E) \\ = \tilde{n}_{\mathbf{k}-\mathbf{q}} [1 - (t_{\mathbf{k}-\mathbf{p}} - t_{\mathbf{k}}) \sum_{\mathbf{p}} \Gamma_{\mathbf{k}-\mathbf{p}}(E)]. \end{aligned} \quad (47)$$

The solution of this integral equation yields the result

$$G_{\mathbf{k}\downarrow}(E) = \left\{ E - t_{\mathbf{k}} + \left[G_{\mathbf{k}\downarrow}^0(E) \right]^{-1} \right\}^{-1} \quad (48)$$

The expressions (44) and (48) were previously derived using the many-electron approach of Hubbard's operators, as described in references [39,40]. It was noted that these results bear resemblance to Anderson's spinons, which also exhibit zero residue in their Green's function. Green's function (44) represents a purely non-quasiparticle state, indicating its unconventional nature. Due to the limited dependence on momentum (\mathbf{k}), the corresponding distribution function of these non-quasiparticle (incoherent) states exhibits low mobility and cannot provide an electrical current.

Regarding Green's function (48), when the doping level $1 - n$ is small, it does not exhibit any poles below the Fermi level (for holes), confirming the previous conclusions. However, as the doping increases, a spin-polaron pole E_F emerges, resulting in the destruction of half-metallic ferromagnetism.

The description of the transition to the saturated state, where the spin-down quasiparticle residue diminishes, resembles that of the Mott transition in the paramagnetic Hubbard model [5]. In this sense, the situation is somewhat comparable to a partial Mott transition occurring in the spin-down subband. For a more detailed discussion on this matter, cf. the review [4] where the orbital-selective Mott transition is explored.

Now we calculate the correction to the magnon frequency. The equation of motion for the spin Green's function reads

$$(\omega - \omega_q) \langle \langle S_q^+ | S_{-q}^- \rangle \rangle_\omega = 2 \langle S^z \rangle + \sum_{\mathbf{k}\mathbf{p}} (t_{\mathbf{k}-\mathbf{q}} - t_{\mathbf{k}}) \Lambda_{\mathbf{k}\mathbf{q}\mathbf{p}}(\omega), \quad (49)$$

$$\Lambda_{\mathbf{k}\mathbf{q}\mathbf{p}}(E) = \langle \langle S_{\mathbf{k}+\mathbf{q}-\mathbf{p}}^+ f_{\mathbf{p}\uparrow}^\dagger f_{\mathbf{k}\uparrow}^\dagger | S_{-\mathbf{q}}^- \rangle \rangle_\omega \quad (50)$$

In the same manner, we derive the integral equation

$$\begin{aligned} & (\omega - t_{\mathbf{k}} + t_{\mathbf{p}} - \omega_{\mathbf{k}+\mathbf{q}-\mathbf{p}}) \Lambda_{\mathbf{k}\mathbf{q}\mathbf{p}}(\omega) \\ &= \delta_{\mathbf{k}\mathbf{p}} \tilde{n}_{\mathbf{k}} + \sum_{\mathbf{r}} (t_{\mathbf{k}+\mathbf{r}+\mathbf{q}-\mathbf{p}} - t_{\mathbf{r}}) \Lambda_{\mathbf{r}\mathbf{q}\mathbf{p}}(\omega). \end{aligned} \quad (51)$$

Neglecting the integral term (which is possible to leading order in the inverse nearest-neighbor number) we obtain from the expansion of the Dyson equation, the renormalized magnon frequency

$$\Omega_{\mathbf{q}} = \omega_{\mathbf{q}} + \sum_{\mathbf{k}} (t_{\mathbf{k}-\mathbf{q}} - t_{\mathbf{k}}) \tilde{n}_{\mathbf{k}}. \quad (52)$$

The exact solution of Equation (51) provides accurate results to leading order in doping, in agreement with the consideration by Nagaoka [41] (see also [39]).

4.3. Antiferromagnetic Case: Small and Large Fermi Surfaces

With the increase in doping, the Nagaoka ferromagnetic state becomes unstable. The instabilities can also be treated within the Kotliar–Ruckenstein representation, as was performed numerically in refs. [42,43]. This representation, adopted above for the ferromagnetic phase (43), is expected to hold also in the antiferromagnetic state when being written down in the local (rotating) coordinate system. Moreover, it will work also in systems with strong spin fluctuations and short-range order (e.g., in the singlet RVB state), but not in the usual structureless paramagnetic state.

The representation (43) is formally very similar to the representation of the Fermi dopons $d_{i\sigma}^\dagger$ [13,44] introduced to describe the formation of small and large Fermi surfaces in doped two-dimensional cuprates. This has the form

$$\tilde{c}_{i-\sigma}^\dagger = -\frac{\sigma}{\sqrt{2}} \sum_{\sigma'} d_{i\sigma'}^\dagger (1 - n_{i-\sigma'}) [S \delta_{\sigma\sigma'} - (\mathbf{S}_i \boldsymbol{\sigma}_{\sigma'\sigma})]. \quad (53)$$

where $\sigma = \pm$, $n_{i\sigma} = d_{i\sigma}^\dagger d_{i\sigma}$, and both Fermi spinon (Abrikosov) and Schwinger boson representations can be used for localized $S = 1/2$ spins. The latter representation has the advantage that the hybridization of spinons with dopons can describe the formation of the large Fermi surface, including the localized states.

On the other hand, the Bose version [13] can successfully describe the small Fermi surface. The presence of strong antiferromagnetic correlations leads to the hopping of dopons between nearest neighbors being strongly suppressed owing to a local antiferromagnetic order [13,44]. The small hole pockets of the Fermi surface, characteristic for the cuprates, are formed, which tend to the $(\pi/2, \pi/2)$ point of the Brillouin zone with increasing the short-range order [13].

Thus, we can apply our representation (43) to the same problem. Note that the description in terms of bosons p (representation (39)) turns out to be oversimplified and incomplete, unlike the approach based on (43), which provides a description in terms of true spin degrees of freedom.

At first sight, the dopon representation can seem to be quite different from standard slave-boson representations. However, the connection can be established by using the constraint $\sum_{\sigma} f_{i\sigma}^{\dagger} f_{i\sigma} \simeq 1$ (which holds at small doping) and the Abrikosov representation for spin operators

$$S_i^z = \frac{1}{2}(f_{i\uparrow}^{\dagger} f_{i\uparrow} - f_{i\downarrow}^{\dagger} f_{i\downarrow}), S_i^{\sigma} = f_{i\sigma}^{\dagger} f_{i-\sigma}. \quad (54)$$

We rewrite (53) as

$$\tilde{c}_{i\sigma} = \frac{1}{2}(d_{i\downarrow}^{\dagger} f_{i\uparrow}^{\dagger} - d_{i\uparrow}^{\dagger} f_{i\downarrow}^{\dagger}) f_{i\sigma}. \quad (55)$$

Then, we can introduce Anderson's Bose holon operator as a singlet combination of Fermi spinon and new dopon operators [16,44],

$$e_i = f_{i\uparrow} d_{i\downarrow} - f_{i\downarrow} d_{i\uparrow}. \quad (56)$$

Thus, we return to Anderson's representation (4), except for the difference in the factor of $1/\sqrt{2}$. The problem with this factor does not take place in our version of the Kotliar–Ruckenstein representation (43) due to the factor of M in (17). Note that the dopon representation can be also derived in the many-electron approach of Hubbard's operators using the analogy with the equivalent narrow-band $s-d$ exchange model [20,45].

5. Discussion

We have demonstrated that the Kotliar–Ruckenstein representation [8] provides a unified description of paramagnetic and magnetic phases. In the paramagnetic phase, we present a new interpretation in terms of spin–charge separation and conservation of the Fermi surface in the insulator state. We have also performed the derivation of the Hamiltonian in the magnetically ordered phase in the spin–wave region, which enables one to obtain an agreement with well-established results for the ferromagnetic case.

The constructed approach is somewhat similar to the Holstein–Primakoff representation for Heisenberg systems. The Kotliar–Ruckenstein representation includes both Fermi and Bose (or spin) operators and has a rather complicated structure with radicals. Therefore, in a sense, it solves the problem of describing transmutation statistics of auxiliary particles when passing from spin–liquid to magnetic phase, which was discussed in Section 2 and formulated earlier as an important issue (see, e.g., ref. [12]).

Under deconfinement conditions, the characteristics of the energy spectrum are significantly affected by the presence of spinon excitations, and this should result in their pronounced dependence on temperature on the scale of the Heisenberg interaction, which can be small in comparison with bare electron energies. The corresponding expressions for Green's functions can be applied to write down the optical conductivity and describe the optical transitions between Hubbard's subbands, as demonstrated in ref. [19].

Anderson [6] applied the concept of spinons to explain the linear specific heat in copper-oxide systems by the contribution of gapless spinons forming the Fermi surface in the spin–liquid-like uniform resonating valence bond (RVB) state. Although for the cuprates, this point remains highly debatable, there exists experimental evidence for contributions of spinons (gapless magnetic excitations) to specific heat and thermal conductivity, etc., in some compounds with frustrated lattices (see, e.g., refs. [31,46,47]).

At the same time, in the magnetically ordered phase, we have usual spin-wave excitations. These phases are also successfully described by the Kotliar–Ruckenstein representation with account of incoherent states. Exotic phases, including both antiferromagnetic order and fractionalized excitations (so-called AFM* or SDW* phase [4,48]), can be considered too. In systems with magnetic or superconducting ground states, there is still a

possibility for a spin–liquid-like state to emerge at intermediate temperatures, particularly in systems with frustration [48].

As we have demonstrated, topological transitions of a different nature with a reconstruction of the Fermi surface occur in antiferromagnetic and ferromagnetic [17] phases. It is evident now that the Mott transition leading to a non-magnetic ground state is closely linked to topological characteristics. This transition involves a deconfined spin–liquid state that exhibits fractionalization and extensive quantum entanglement [10]. Understanding the exotic correlated paramagnetic phase, which can possess intricate structures, is a significant challenge in this context.

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