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Doped Carrier Formulation of the t–J model: Monte Carlo Study of the Anisotropic Case

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We derive a doped carrier representation of the t–J model Hamiltonian. Within this approach the t–J model is described in terms of holes hopping in a lattice of correlated spins, where holes are the carriers doped into the half-filled Mott insulator. This representation of the t–J Hamiltonian is very convenient for underdoped systems since close to half-filling it allows for a controlled treatment of the crucial constraint of no doubly occupied sites. When neglecting the transverse spin–spin interaction, the effective Hamiltonian can be investigated with classical Monte Carlo simulations. We discuss the results obtained for systems consisting of several hundred lattice sites.

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1. Theoretical background

We start with the t–J Hamiltonian on a square lattice [1]:

$$H_{t-J} = -\sum_{ij\sigma} t_{ij} X_i^{\sigma 0} X_j^{0\sigma} + \text{h.c.} + J \sum_{ij} \left(\boldsymbol{Q}_i \boldsymbol{Q}_j - \frac{1}{4} n_i^{\mathrm{P}} n_j^{\mathrm{P}} \right), \tag{1}$$

where we have introduced a set of the on-site Hubbard operators $X^{ab} := |a\rangle\langle b|$, $a, b = 0, \uparrow, \downarrow$, and $n_i^{\mathrm{P}} = X_i^{\uparrow\uparrow} + X_i^{\downarrow\downarrow}$. Here, $\boldsymbol{Q}_i = \frac{1}{2} \sum_{\sigma\mu} X_i^{\mu 0} \boldsymbol{\tau}_{\mu\sigma} X_i^{0\sigma}$ with $\boldsymbol{\tau}$ being the Pauli matrices. The local no double occupancy (NDO) constraint is rigorously taken into account at the expense of the introduction of the Hubbard operators with commutation relations more complicated than those of the standard fermion algebra. Although the Q_z, Q^+ and Q^- operators formally fulfill the

commutation relations of the spin SU(2) algebra, away from half-filling they do not correspond to the true spin degrees of freedom. This is because $\boldsymbol{Q}^2$ (the Casimir operator) that in the standard case labels the SU(2) representations and is equal to a c-number, $s(s+1)_{s=1/2} = 3/4$, now takes the form $\boldsymbol{Q}^2 = \frac{3}{4}n^{\mathrm{P}}$. In a general case, the operators $\boldsymbol{Q}$ transform themselves in the representations of a group bigger than SU(2), namely, in those of its supersymmetric extension, SU(2|1). Physically, this means that the charge and spin degrees of freedom are mixed up in multiplets under the SU(2|1) action.

In the present paper we use a representation of the t–J model where the electron spin operator can be cast under some restrictions into the form [2]:

$$\boldsymbol{Q} = \boldsymbol{S} + \boldsymbol{M}. \tag{2}$$

Here, $\boldsymbol{S}$ is the SU(2) spin operator ($\boldsymbol{S}^2 = 3/4$) whereas $\boldsymbol{M}$ is the spin operator of the doped holes. This relation can be established only in the Gutzwiller projected Hilbert space. Thus, from the very beginning it must be appreciated that the imposing of the NDO constraint by making use of the Hubbard operator representation of the t–J model, leads naturally to the theory with the SU(2) spinons and doped carriers, instead of the lattice electrons in more conventional approaches. This new representation seems to be quite appealing, since the NDO constraint states now that the states with two holes on a site are excluded. In the physically interesting region of low doping, $\delta = 1 - n \ll 1$, this constraint may therefore be safely relaxed. This is in a sharp contrast to the conventional, e.g., slave-boson type approaches which apply the NDO constraint directly to the lattice electrons. In the latter case, close to half-filling $n_i \approx 1$ and that constraint becomes of the crucial importance.

Since there is one-to-one correspondence between the generators of a compact simple (super)algebra and their coherent-state (CS) symbols, we can deal directly with the SU(2|1) CS symbols of the Hubbard operators. Acting with the "lowering" superspin operators $X^{\downarrow\uparrow}$ and $X^{\downarrow 0}$ on the "highest weight" state $|\uparrow\rangle$ we get the normalized SU(2|1) coherent state in the 3D fundamental representation, $|z,\xi\rangle = (1+\bar{z}z+\bar{\xi}\xi)^{-1/2}\exp\left(zX^{\downarrow\uparrow} + \xi X^{0\uparrow}\right)|\uparrow\rangle$. Here, z is a complex number, and ξ is a complex Grassmann parameter. The Grassmann parameter appears here due to the fact that $X^{\downarrow 0}$ is a fermionic operator in contrast to the bosonic operator $X^{\downarrow\uparrow}$. The product $\xi X^{0\uparrow}$ represents therefore a bosonic quantity as required. At $\xi = 0$, the SU(2|1) CS reduces to the ordinary SU(2) CS, $|z,\xi = 0\rangle \equiv |z\rangle$, parametrized by a complex coordinate $z \in \mathrm{CP}^1$. In contrast, at $z = 0$ it represents a pure fermionic CS. The fact that the SU(2|1) CS's incorporate both the spin SU(2) CS's and the pure fermionic CS's is of central importance for the derivation of the basic Eq. (2). Then, we get the CS symbols

$$X^{0\downarrow}_{\mathrm{cl}} = -\frac{z\bar{\xi}}{1+|z|^2}, \qquad X^{0\uparrow}_{\mathrm{cl}} = -\frac{\bar{\xi}}{1+|z|^2},$$

$$Q^+_{\rm cl} = \frac{z}{1+|z|^2}\left(1-\frac{\bar\xi\xi}{1+|z|^2}\right), \qquad Q^z_{\rm cl} = \frac{1}{2}\frac{1-|z|^2}{1+|z|^2}\left(1-\frac{\bar\xi\xi}{1+|z|^2}\right), \tag{3}$$

where $A_{\rm cl} := \langle z,\xi|A|z,\xi\rangle$ for arbitrary operator A. Introducing the notation

$$\bar\psi_\uparrow = \frac{z\bar\xi}{1+|z|^2}, \qquad \bar\psi_\downarrow = -\frac{\bar\xi}{1+|z|^2}, \tag{4}$$

we get

$$Q^+_{\rm cl} = S^+_{\rm cl} + \bar\psi_\uparrow\psi_\downarrow, \qquad Q^z_{\rm cl} = S^z_{\rm cl} + \frac{1}{2}(\bar\psi_\uparrow\psi_\uparrow - \bar\psi_\downarrow\psi_\downarrow),$$
$$n^{\rm P}_{\rm cl} = 1 - (\bar\psi_\uparrow\psi_\uparrow + \bar\psi_\downarrow\psi_\downarrow). \tag{5}$$

At this stage we find it convenient to introduce the CS symbol of the spin operator of the doped carriers, $\boldsymbol{M}_{\rm cl} = \sum_\sigma \psi^+_\sigma \boldsymbol{\tau}_{\sigma\sigma'}\psi_\sigma$, which transforms as a true SU(2) vector. With this notation the representation (2) is an immediate consequence of (5). After some algebra the Lagrangian of the t–J model can be written in the form

$$L = \sum_{i\sigma}\langle\psi_{i\sigma}|(-\partial_t)|\psi_{i\sigma}\rangle + \sum_i\langle z_i|(-\partial_t)|z_i\rangle + \sum_{ij\sigma} t_{ij}\bar\psi_{i\sigma}\psi_{j\sigma}$$
$$+{\rm h.c.} + L_{\boldsymbol{SM}}, \tag{6}$$

where $|z\rangle$ stands for the SU(2) CS, $|\psi_\sigma\rangle = (1+\bar\psi_\sigma\psi_\sigma)^{-1/2}\exp(\psi_\sigma\Psi^\dagger_\sigma)|0\rangle$ denotes the fermionic CS and

$$L_{\boldsymbol{SM}} = -J\sum_{ij}\left[\left(\boldsymbol{S}^{\rm cl}_i\boldsymbol{S}^{\rm cl}_j - \frac{1}{4}\right)\right.$$
$$\left. + \left(\boldsymbol{S}^{\rm cl}_i\boldsymbol{M}^{\rm cl}_j + \boldsymbol{S}^{\rm cl}_j\boldsymbol{M}^{\rm cl}_i\right) + \left(\boldsymbol{M}^{\rm cl}_i\boldsymbol{M}^{\rm cl}_j - \frac{1}{4}\widehat{\delta}^{\rm cl}_i\widehat{\delta}^{\rm cl}_j\right)\right].$$

Two extra degrees of freedom that appear in (6) with respect to the basic fields z and ξ in Eq. (3) are taken care of by the constraint $\boldsymbol{M}_{\rm cl} = -\boldsymbol{S}_{\rm cl}\hat\delta_{\rm cl}$. Finally, the quantum Hamiltonian that corresponds to (6) reads

$$H_{t-J} = \sum_{ij\sigma} t_{ij}\,\Psi^+_{i\sigma}\Psi_{j\sigma} + {\rm h.c.} + J\sum_{ij}\left[\left(\boldsymbol{S}_i\boldsymbol{S}_j - \frac{1}{4}\right)\right.$$
$$\left. + (\boldsymbol{S}_i\boldsymbol{M}_j + \boldsymbol{S}_j\boldsymbol{M}_i) + \left(\boldsymbol{M}_i\boldsymbol{M}_j - \frac{1}{4}\widehat{\delta}_i\widehat{\delta}_j\right)\right]. \tag{7}$$

2. Numerical results for anisotropic case

Although the representation (7) of the t–J model is exact, it can be diagonalized only for small systems. Then, however, one could carry out the same calculations for the original formulation of the t–J model. Our aim is to perform approximate calculations for sufficiently larger systems, when the finite-size effects become negligible. In order to be able to do it, we consider anisotropic case neglecting operators S^+ and S^- (t–J_z model). The remaining S^z operators commute with all other quantities, and they can be replaced by their

eigenvalues. When calculating the partition function, we sum up over all possible configurations of S_i^z. The z-component of the constraint $\boldsymbol{M}_i = -\delta_i \boldsymbol{S}_i$ can exactly be taken into account through introducing the Lagrange multiplier: $\lambda \sum_i \left[(\frac{1}{2} + S_i^z)\, \Psi_{i\uparrow}^\dagger\, \Psi_{i\uparrow} + (\frac{1}{2} - S_i^z)\, \Psi_{i\downarrow}^\dagger\, \Psi_{i\downarrow} \right]$, with $\lambda \to \infty$. In the numerical calculations we have taken $\lambda = 100t$. This simplified constraint preserves the physical meaning of the exact one, since sites with $S^z = \sigma$ are empty or occupied by a dopant particle with spin $-\sigma$. Double occupancy is excluded, since it would lift the energy by λ. The resulting Hamiltonian can be analyzed withing the Monte Carlo algorithm described in Ref. [3]. The simulations have been carried out on a 20×20 system with first (t) and second nearest neighbor $t' = -0.5t$ hopping integrals. $J = 0.4t$ and $k_{\mathrm{B}}T = 0.1t$ have been assumed. For systems of such a size the finite size effects are negligible as can be inferred from Fig. 20 in Ref. [3].

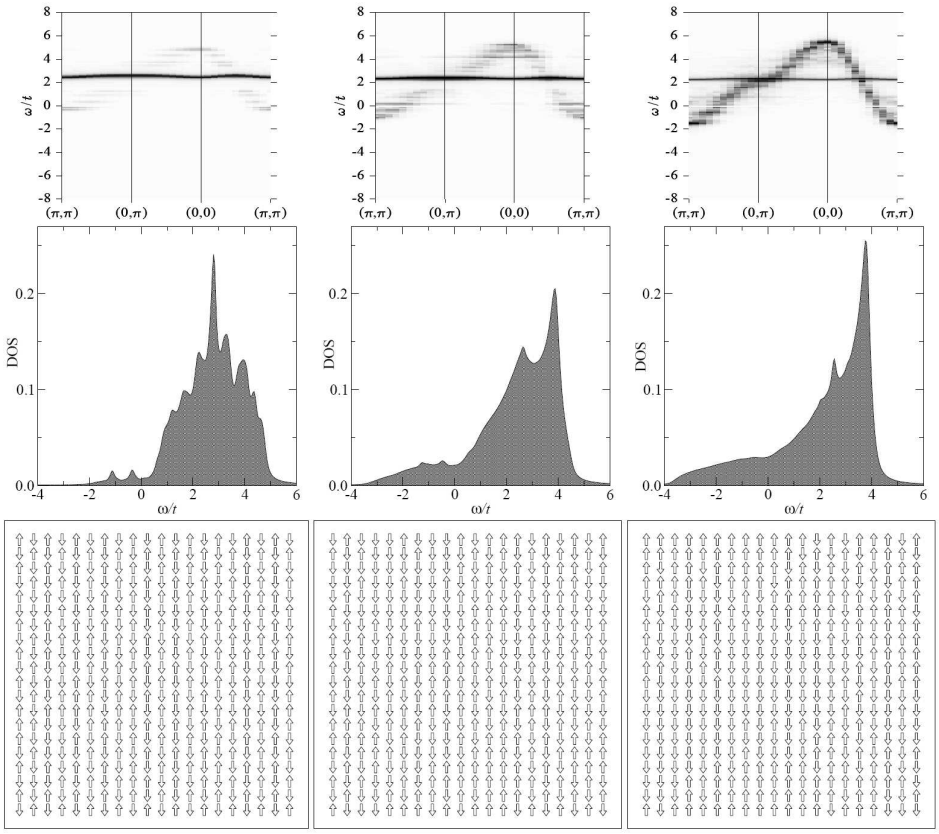

Fig. 1. The upper parts show the hole spectral functions calculated along the symmetry lines of the Brillouin zone. Chemical potential is located at the zero energy. The middle ones show the density of states. The lower ones show typical snapshots for the spinon (S^z) configurations in the Monte Carlo simulations. Left, middle, and right parts correspond to $\delta = 0.025, 0.1$ and 0.15, respectively.

Results presented in Fig. 1 clearly indicate that the spectral properties of the dopant particles are very different from those of the free electron gas. This difference is especially pronounced in the strongly underdoped regime, where the most of the spectral weight occurs at positive energies for all momentum states. This clearly indicates on the absence of well defined quasiparticles. It is interesting that even for a relatively large doping $\delta \approx 0.15$ the spectral functions still do not resemble the δ-like functions. Other interesting feature shows up in the density of states. In the underdoped regime, a pseudogap opens at the Fermi energy. This gap vanishes for large concentration of carriers ($\delta > 0.15$). One can see that the structure of the density of states strongly depends on doping, which is a hallmark of strongly correlated systems. Finally, we briefly discuss the influence of doping on the antiferromagnetic order. For vanishing doping there is a long--range antiferromagnetic order. For larger doping the long-range order vanishes, however, a short-range antiferromagnetic order remains. Finally, for $\delta \approx 0.15$ antiferromagnetic correlations disappear. At this concentration the pseudogap in the density of states disappears as well. Our approach does not require translational symmetry and, therefore, can straightforwardly be extended to take into account inhomogeneities [4], which seem to play an important role in hight temperature superconductors.

Acknowledgments

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