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Phase separation in the $U = \infty$ one-band Hubbard model

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Abstract. We study the ground state of the $U = \infty$ one-band SU(N) Hubbard model on a square lattice in the leading order of a $1/N$ expansion using a Baym–Kadanoff expansion and the X-operator formulation. We find that the homogeneous paramagnetic solution can become unstable against phase separation due to next-nearest-neighbour hopping.

Since the discovery of high-T_c superconductors [1] there has been renewed interest in the investigation of strongly correlated Fermi systems. The two-dimensional one-band Hubbard model [2, 3], as one of the simplest models, has been suggested [4] to be a good starting point for a description of correlations in the CuO planes of cuprate-based high-T_c superconductors. Several approximations have been used to study its behaviour for small, intermediate and large values of the Hubbard repulsion U [5]. Here we restrict our calculations to the $U = \infty$ limit of the Hubbard model. Moreover, in order to use controlled expansions, we consider the limit of large spin degeneracy N, which allows an expansion in the small parameter $1/N$. Calculations have already been carried out for the case $U = \infty$, using the slave-boson (SB) method [6] and alternatively the X-operator technique [7]. For $N = \infty$ one gets a paramagnetic solution. One important topic of recent research is the investigation of phase separation [8, 9] in various models. For the $U = \infty$ one-band Hubbard model, considered here, Kotliar and Liu [6] have shown that for $N \to \infty$ the homogeneous paramagnetic phase is stable against phase separation for all fillings. Doing this, they restricted themselves to nearest-neighbour (NN) hopping only. So one should ask whether this stability is a special feature of this restriction, corresponding to a symmetric form of the density of states in the uncorrelated system. As an example in which the density of states is no longer symmetric one can consider an additional next-nearest-neighbour (NNN) hopping. Moreover the latter is important, in order to make possible the description of the Fermi surface of the CuO layers in some compounds by a simple tight-binding model [10–13].

In this work we will show that for $N \to \infty$ the homogeneous paramagnetic solution may become unstable against phase separation [14] even for an infinitesimal amplitude of the NNN hopping matrix element. To this end we use the X-operator [16] formulation and the Baym–Kadanoff perturbation expansion [7, 17] to determine the single-particle Green's function (GF).

The Hamiltonian under consideration has the form

$$H = \sum_{\substack{p=1,N \\ i}} E_{ip} X_i^{pp} + \sum_{\substack{p=1,N \\ ij}} \frac{t_{ij}}{N} X_i^{p0} X_j^{0p} \tag{1}$$

where i stands for the lattice site, and E_{ip} for atomic energies; $p = 0$ denotes the unoccupied and $p = 1, \ldots, N$ the singly occupied orbitals with spin index p. We thus have extended

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the original SU(2) model with two spin states to an SU(N) model with N spin states. The Hubbard operators X_i^{pq} with $p = 0, q = 0$ or $p > 0, q > 0$ have bosonic character whereas the operators with $p = 0, q > 0$ or $p > 0, q = 0$ have fermionic character. They obey the following commutation and anticommutation rules, respectively:

$$[X_i^{pq}, X_j^{rs}]_{\mp} = \delta_{ij}(\delta_{qr} X_i^{ps} \mp \delta_{sp} X_i^{rq}). \tag{2}$$

The first term in equation (1) describes isolated atoms, the second one the hopping between atoms with matrix elements t_{ij}. The scaling factor N has been introduced, so the limit $N \to \infty$ is non-trivial, i.e. atomic and kinetic energy are of the same order in N. The X-operators act within a Hilbert space defined by the constraint [18]

$$\sum_{p=0}^{p=N} X_i^{pp} = \frac{N}{2} \tag{3}$$

which is equivalent to that usually used in slave-boson formulations of the problem [6].

We use the notation $X_{i_1}^{p_1 q_1}(\tau_1) \equiv X(1)$ and add a source term H_s to the Hamiltonian to define single-particle nonequilibrium thermal Green's functions:

$$G(11') = \langle\langle X(1) X^{\dagger}(1')\rangle\rangle = \frac{-\langle T S X(1) X^{\dagger}(1')\rangle}{\langle S\rangle}. \tag{4}$$

Here, $X(1)$ and $X(1')$ are fermionic X-operators in the Heisenberg representation, $\langle \ldots \rangle$ is the thermal average, T the imaginary-time ordering operator and

$$S = T \exp\left(-\int_0^{\beta} \mathrm{d}\tau_1 \; H_s(\tau_1)\right). \tag{5}$$

The source term has the form

$$H_s(\tau_1) = -\int \mathrm{d}2 \; \delta(\tau_2 - \tau_1)\, X(2) K(2) \tag{6}$$

where sources K are introduced with respect to bosonic X-operators only. Writing down the equation of motion for the single-particle GFs one gets higher-order GFs, which can be expressed in terms of appropriate functional derivatives of the single-particle GFs with respect to the source K [7, 17]. In addition, one can express the GFs appearing in the equation of motion in terms of the self-energy Σ and express Σ in terms of functional derivatives [7, 17]. On this basis it is possible to carry out a controlled $1/N$ expansion for G, Σ and the expectation values of bosonic X-operators [19–21]. In the leading order, i.e. for $N \to \infty$, the self-energy is frequency independent, so one obtains an effective uncorrelated band with a dispersion determined by a renormalization of the hopping term and a shift of the atomic energy as given below; see equation (10).

Searching for instability against phase separation one has to determine the chemical potential μ as a function of the mean occupation number N_0,

$$N_0 = \sum_{\substack{p=1 \\ i}}^{p=N} \langle X_i^{pp}\rangle. \tag{7}$$

Restricting oneself to the case where $T = 0$, one can use the relation

$$\frac{\partial\langle H\rangle}{\partial N_0} = \mu. \tag{8}$$

Inserting the Hamiltonian (1) we obtain

$$\langle H\rangle = \Delta \sum_{\boldsymbol{k}} t(\boldsymbol{k}) \Theta(\mu - \epsilon(\boldsymbol{k})) \tag{9}$$

for the leading order in the $1/N$ expansion. Here we have set the atomic energies equal to zero; $\epsilon(\boldsymbol{k})$ denotes the renormalized single-particle energies which are spin independent and given by

$$\epsilon(\boldsymbol{k}) = \lambda + \frac{\Delta}{N} t(\boldsymbol{k}) \tag{10}$$

with the shift of the atomic energy

$$\lambda = -\frac{1}{N_s} \sum_{\boldsymbol{k}'} t(\boldsymbol{k}') \Theta(\mu - \epsilon(\boldsymbol{k}')) \tag{11}$$

and the renormalization factor $\Delta = \langle X_i^{00} \rangle$, where the homogeneous case is assumed. Above, $t(\boldsymbol{k})$ is the Fourier transform of t_{ij}, N_s is the number of sites and Θ the step function. Using the constraint (3) one has

$$\frac{\Delta}{N} \equiv \alpha = \frac{1}{2} - \frac{N_0}{N_s N}. \tag{12}$$

Note that all values have to be calculated in their leading order, e.g. $\langle X^{00} \rangle$ in O(N) and λ in O(1). Not paying attention to this would lead to a mixing of different orders in $1/N$. The above equations (9)–(12) agree with those as obtained for $N \to \infty$ in the well-established SB treatment [6].

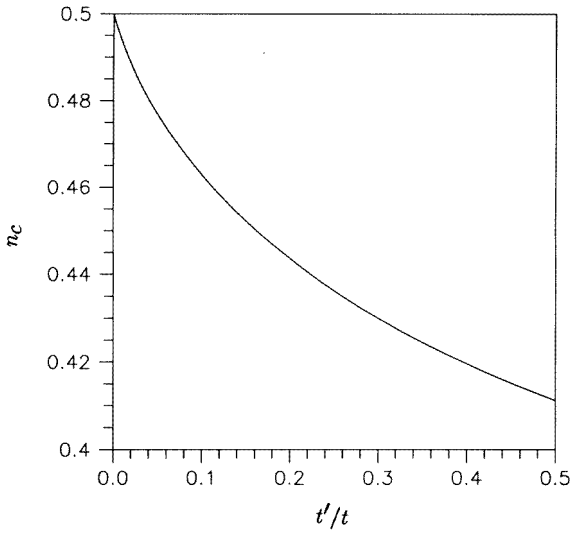

Figure 1. The critical density n_c per spin degree of freedom as a function of the NNN hopping amplitude t'/t for $t > 0$ according to equation (18). For n_c the l.h.s. of (15) is zero, i.e., the inverse compressibility diverges.

On introducing

$$y = (\mu - \lambda)/\alpha \tag{13}$$

equation (8) becomes

$$\mu = \lambda - \frac{\alpha^2}{N_s} \sum_{\boldsymbol{k}} t(\boldsymbol{k})\, \delta(\epsilon(\boldsymbol{k}) - \mu)\, \frac{\partial y}{\partial \alpha}. \tag{14}$$

Stability against phase separation requires

$$\frac{\partial \mu}{\partial n_p} > 0 \tag{15}$$

in which n_p is the density per spin, related to N_0 (equation (7)) by $N_0 = N_s N n_p$ in the homogeneous paramagnetic case. Inserting equation (14) into the relation (15) leads to

$$1 - \frac{2y}{\alpha} n_p^{(0)}(y) > 0 \tag{16}$$

as a condition for the stability of the homogeneous solution with the energy dispersion according to equations (10) and (11). In equation (16), $n_p^{(0)}$ is the unperturbed density of states per spin direction, i.e., calculated with $\lambda = 0$, $\Delta/N \equiv \alpha = 1$ in equation (10); α is determined via equations (12) and (7) by $\langle X^{pp} \rangle$. Note that because of the constraint (3) some projection properties of the X-operators, e.g. $X_i^{00} X_i^{00} = X_i^{00}$, get lost [20]. As a result, relations such as $X_i^{pq} = X_i^{p0} X_i^{0q}$ which are usually used to express expectation values of bosonic X-operators in terms of Green's functions as, e.g., $\langle X_i^{pp} \rangle = -\langle T X_i^{0p}(\tau) X_i^{\dagger 0p}(\tau^+) \rangle$, are no longer valid. The latter relation has to be replaced by a more complicated one; the derivation for arbitrary temperature is, even for the leading order, a bit cumbersome [20]. However, restricting oneself to the case where $T = 0$, one can determine the density n_p per spin degree of freedom via equation (8), leading to

$$n_p = \int_{-\infty}^{y} \mathrm{d}\epsilon \; n_p^{(0)}(\epsilon). \tag{17}$$

Let us show now that the condition (16) no longer needs to be fulfilled for all densities if a NNN hopping is included in t_{ij}. Considering NN hopping exclusively, one finds that an instability can occur only for a density per spin $n_p = 0.5$, i.e.,

$$\sum_{p=1}^{p=N} \langle X_i^{pp} \rangle = N/2.$$

Thus in this case no phase separation can occur due to the constraint (3). Permitting NNN hopping, one can get some $n_p(y = 0) < 0.5$, leading to an instability with $y > 0$ and $n_p(y) < 0.5$. This follows from

$$\alpha = \frac{1}{2} - n_p = \frac{1}{2} - \int_{-\infty}^{y} \mathrm{d}\epsilon \; n_p^{(0)}(\epsilon)$$

and the positivity of the unperturbed density of states, $n_p^{(0)}(\epsilon)$. Note that due to the inclusion of the NNN hopping, $n_p^{(0)}(\epsilon)$ is no longer symmetric and

$$\int_{-\infty}^{0} \mathrm{d}\epsilon \; n_p^{(0)}(\epsilon) \gtrless 0.5$$

becomes possible, depending on the sign of the NNN hopping amplitude. To fix the ideas we considered the energy dispersion

$$t(\boldsymbol{k}) = 2t[\cos(k_x) + \cos(k_y)] - 4t'[\cos(k_x)\cos(k_y)] \tag{18}$$

in which the lattice spacing is set to unity. We solved equations (16) and (17) numerically to determine the critical density n_c per spin for which the l.h.s. of the relation (16) is zero, i.e., the inverse compressibility diverges [22]. Figure 1 shows this critical density as a function of the NNN hopping amplitude t' ($t', t > 0$), for which the physically relevant parameter range is chosen according to [10, 12]. Due to the constraint $n_p \leqslant 0.5$, only positive ratios

t'/t of both hopping amplitudes lead to an instability for $t > 0$, corresponding to the hole picture. In contrast, for the electron picture in which $t < 0$, an instability occurs only for $t'/t < 0$.

The hole picture of the model with infinite Coulomb interaction U, considered here, implies the exclusion of double occupancy of the *holes* for $N = 2$. Thus in the hole picture only electron doping with respect to the half-filled model is possible. If $t'/t > 0$, i.e., phase separation can occur, the form of the Fermi surface for the $N \to \infty$ result of our model agrees qualitatively with that experimentally found for electron-doped $Nd_{2-x}Ce_xCuO_4$ [13, 24].

To explain why in the case with inclusion of NNN hopping phase separation can occur whereas in the NN hopping case this is not possible, one has to look at equation (16). This equation shows that the filling-dependent shift λ of the single-particle energies plays an important role, because it determines the value of $y = (\mu - \lambda)/\alpha$. In the case of NN hopping only and putting the unrenormalized atomic energy to zero, $\mu < \lambda$ holds in the less-than-half-filled case; thus $y < 0$.

This picture changes if NNN hopping is switched on. Because the band is not symmetric (with respect to the function $n_p^{(0)}(\epsilon)$), one can have $\mu > \lambda$ in the half-filled case, i.e., the chemical potential lies above the renormalized atomic energy. This is the main difference between the two cases, with and without NNN hopping, and leads to the possibility of phase separation in the former case. One should note that for the $U = \infty$ one-band Hubbard model in the limit $N \to \infty$ neither magnetic phases nor superconductivity occur [20]; thus the instability of the homogeneous paramagnetic solution against phase separation, discussed here, is the only one. This can change if a Heisenberg (J-) term is introduced into the Hamiltonian, i.e., the t–J-model is considered instead of the t-model (i.e., the $U = \infty$ model).

Grilli, Castellani and Kotliar [26] have investigated the t–J-model in the large-N limit using a decoupling for the magnetic part and considering NN hopping only. They find phase separation for zero J only in the half-filled case. This is in agreement with results of numerical investigations as well as analytical considerations [15]. Psaltakis and Papanicolaou [27] have considered an additional NNN hopping in the t–J-model (i.e., the t–t'–J-model) finding phase separation for zero J. They used a $1/N$ approach, too; however, they altered the commutation relations of the Hubbard operators in an *uncontrolled* way. Deeg and Fehske [28] have considered the t–t'–J-model finding phase separation for $J = 0$, $t' = 0$ only for the half-filled case, whereas for the cases where $t' = 0$, $J \neq 0$ and $t' \neq 0$, $J \neq 0$ that were also investigated phase separation occurs for a less-than-half-filled system. The case where $J = 0, t' \neq 0$ has not been considered explicitly. The method that the authors used is the $N = 2$ saddle-point approximation of the slave-boson functional integral representation for the partition function. It should be emphasized that for $N = 2$ this approximation is not controlled by a small parameter; thus it does not correspond to the saddle-point solution in the large-N case, which becomes exact for $N \to \infty$. In contrast to the former results we get phase separation within an controlled expansion even in the absence of a Heisenberg (J-) term.

In conclusion, we have shown that even for the simple two-dimensional $U = \infty$ one-band Hubbard model (i.e., the t–J-model with zero J) in the limit $N \to \infty$ phase separation can occur, which usually is thought to require more complicated models with additional short-range interactions [29] such as, e.g., a Heisenberg (J-) term. In the model considered here we find, using parameters from band-structure calculations, that only the electron-doped and not the hole-doped system can become unstable against phase separation near half-filling.

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