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A renormalization-group study of the t–J model

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Abstract. The t–J model has been proposed to describe the physics of copper oxide planes in high-temperature superconductors. A real-space quantum renormalization-group method is developed in order to study the t–J Hamiltonian in a square lattice. The zero-temperature phase diagram is analysed for electron concentrations near the half-filled band and ratio J/t. A critical line is found that separates two distinct regions: one of a gas of holes in an antiferromagnetic background, and the other consisting of a phase in which holes segregate into a hole-rich and a pure antiferromagnetic region, as demonstrated by chemical-potential eigenvalue calculations near the phase attractor. The results are close to the experimental observations.

1. Introduction

High-temperature superconductors (HTSC) are the object of intense current research. There is substantial experimental evidence that the conducting carriers have wavefunctions mainly in the CuO_2 plane and, therefore, a single plane may be independently studied. Another important observation is that the parent compounds, such as La_2CuO_4 and $YBa_2Cu_3O_6$, are antiferromagnetic insulators with the copper sites in a $3d^9$ configuration (Cu^{2+}) [1]. When electrons or holes are introduced into the CuO planes by doping, the antiferromagnetic long-range order is gradually destroyed, and eventually a superconducting state becomes observable at a critical doping value. The exact manner in which these processes come about is of central importance to understand the physics of HTSC. It has been suggested earlier [2] that the simplest model to deal with this problem is the 2D single-band Hubbard model, i.e. a model that includes only one orbital per CuO_2 unit. More recently, the t–J model [3] has also been proposed in order to explain how the magnetic order gives way to superconductivity. This model may be derived either as the strong-coupling ($U/t \gg 1$) limit [4] of the Hubbard model or directly from a Cu–O two-band Hamiltonian [2, 3].

It is a general belief that the Hubbard and the t–J Hamiltonians are the most basic models that may be used to describe the strongly correlated electrons in the CuO planes. Therefore, it is worthwhile to determine first their general properties, before the introduction of more sophisticated models. However, both models with parameter spaces relevant to HTSC are difficult to treat and there are no exact solutions in 2D. Consequently many different techniques have been used, such as variational Monte Carlo, quantum Monte Carlo, slave bosons, exact diagonalization methods and several others [5]. The strategy adopted in many of these works is to concentrate on the low-energy and low-temperature properties.

In this paper we study the zero-temperature phase diagram for the 2D t–J model by means of a real-space quantum renormalization-group (QRG) method. This is a non-perturbative method that requires a truncation of the Hilbert space, which leads to an uncontrolled approximation. However, the block renormalization-group approach has been

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extremely successful and widely used in the study of critical phenomena and the transitions that take place in the ground-state and lower excited-states subspace [6]. Section 2 is very technical and the method is developed by parts, studying limiting situations separately and finishes with the discussion of the t–J model at doping concentration near the half-filled band, i.e. the electron density per site $n \leqslant 1$. In section 3 we investigate the phase separation line for the case of isotropic and anisotropic (Ising) spin–spin coupling. The phase separation problem for the t–J model has attracted considerable attention recently and, consequently, has been studied by different methods with conflicting results [7–9]. Therefore it is a problem not settled yet, and it provided the motivation to perform a real-space QRG calculation to study the critical behaviour of the t–J Hamiltonian. We present our results in section 3 and compare with previous calculations and experimental measurements in HTSC systems. Our conclusions are summarized in section 4.

2. The method

The t–J Hamiltonian is described by a lattice Hamiltonian of localized electrons of spin one-half with antiferromagnetic (AF) Heisenberg exchange interaction (J) between nearest-neighbour spins. Upon doping, electrons are removed, leaving behind a 'hole' or missing spin, which can move through the plane because nearest-neighbour electrons can hop into its place with probability amplitude t. The t–J Hamiltonian may be written as

$$H = -t \sum_{\langle i,j\rangle,\sigma} (C^{+}_{i,\sigma} C_{j,\sigma} + \text{HC}) + \sum_{\langle i,j\rangle} [W(\sigma^x_i \sigma^x_j + \sigma^y_i \sigma^y_j) + J\sigma^z_i \sigma^z_j] - \sum_i (\mu n_i - C) \qquad (1)$$

where $C^{+}_{i,\sigma}$ and $C_{i,\sigma}$ are creation and annihilation operators for an electron of spin σ at site i, with the constraint of no doubled occupancy, $n_i = C^{+}_i C_i$ is the occupation number, t is the hopping amplitude, J the AF exchange interaction ($J > 0$) and $W = J(1 - \Delta)$ with $0 \leqslant \Delta \leqslant 1$. The chemical potential μ controls the concentration of electrons; $\mu = +\infty$ at half-filling (i.e. $n_i \equiv n \equiv 1$) and $\mu = -\infty$ for zero electron density.

In order to explain our procedure, we perform our calculation through the following steps: we begin with the study of the antiferromagnetic Heisenberg system, since it is easier to find proper transformation cells in the pure system. Then we derive how the hopping amplitude is scaled for a single hole motion in these cells. Thirdly, we study the diluted AF magnet without hopping to find how the dilution modifies the recurrence relation for the exchange coupling. Finally we introduce the hopping in the diluted AF magnet and argue that this case corresponds to an annealed magnet at $T > 0$ K. After the analysis of these separate cases, we obtain the recurrence relations for the parameters of the t–J Hamiltonian for densities equal to and below the half-filled band.

2.1. The pure (undoped) antiferromagnet

In the limiting situation $n = 1$, there is one electron per site and the system is clearly governed by the AF spin–spin exchange coupling.

The QRG transformation in 2D is performed in two steps: let us first divide the square lattice of side a into cells of three sites in a row, and the whole crystal Hamiltonian into an intracell part H_0 and an intercell interaction V. Since we are interested in the low-energy properties, we will consider only the (closed) subspace of the (total spin 1/2) states $|+-+\rangle$, $|++-\rangle$ and $|-++\rangle$.

Following a general approach [6], we diagonalize exactly the three-site intracell Hamiltonian; we keep the lowest eigenvalue $E_{-}^{(1)}$ and its corresponding eigenvector (a_1, a_2, a_3). Thus the new renormalized states are defined as

$$|+'\rangle = a_1|+-+\rangle + a_2|++-\rangle + a_3|-++\rangle \tag{2a}$$

$$|-'\rangle = a_1|-+-\rangle + a_2|--+\rangle + a_3|+--\rangle. \tag{2b}$$

In figure 1(a) we show schematically how this first part of the transformation is done. To obtain the new coupling constant J', we write the intercell interactions among the spins of the two cells of figure 1(a). The three interactions are assumed to equal the interaction between two renormalized spins (i and j). In the case of up spins we obtain

$$J' = {}_i\langle +'|_j\langle +'| \sum_{l=1}^{3} J S_{il} \cdot S_{jl} |+'\rangle_j |+'\rangle_i$$

or

$$J' = [3a_1^4 + 3a_2^4 + 3a_3^2 - 2a_2^2a_3^2 - 2a_1^2(a_2^2 + a_3^2)]J \tag{3a}$$

or

$$J' = F(J)J. \tag{3b}$$

For the isotropic case, $W = J$: $a_1 = -2/\sqrt{6}$ and $a_2 = a_3 = 1/\sqrt{6}$; which yields $F(J) = 1$. If $W = 0$, the Ising limit: $a_1 = 1$ and $a_2 = a_3 = 0$; and we find $F(J) = 3$.

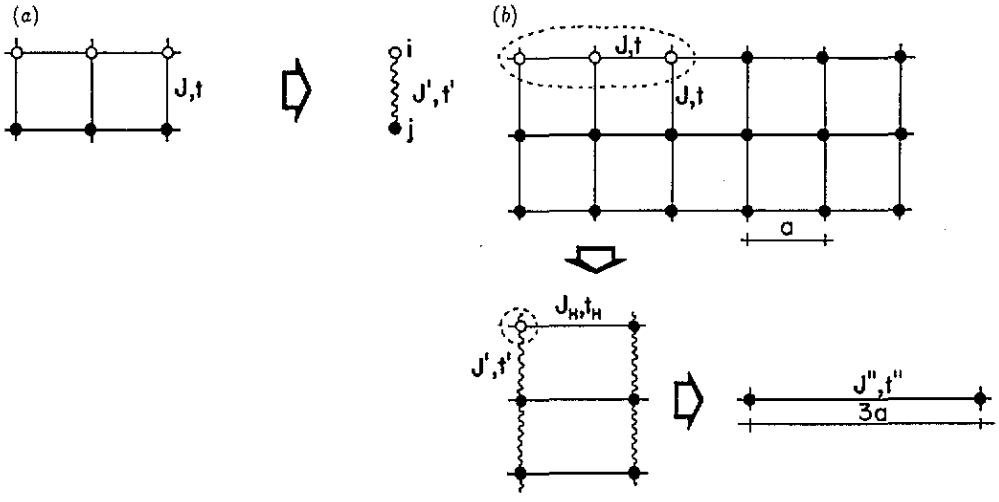

Figure 1. (a) The basic cell has three sites in a row. Two such cells are used to calculate J' and t'. (b) The complete RG transformation. We start with a square lattice of parameter a and, after the transformation, we are left with a square lattice of parameter $3a$. J_H and t_H are equal to J and t for the undoped system.

Next, as the second step (figure 1(*b*)), we extend the RG transformation to the whole lattice; we repeat the same procedure with a $\pi/2$ rotation, as illustrated in figure 1(*b*). This transformation is very similar to that proposed for the Hubbard model [10]. For the undoped system with $n = 1$, $J_H = J$, and after this second transformation, we obtain the final recurrence relation

$$J'' = F(F(J))J. \tag{4}$$

Thus the complete QRG transformation shown in figure 1(*b*) yields $J'' = J$ ($J'' = 3J$) for the AF pure Heisenberg (Ising) system. These results constitute a first test for our real-space QRG procedure because the lower critical dimension for the Heisenberg (Ising) antiferromagnet in a square lattice is $d_c = 2$ (1). At the marginal dimension and at zero temperature, J should not change under iteration and we can expect that $F(J)$ is equal to $b^{(d-d_c)}$, where $d = 2$ is the dimension and $b = 3$ the scaling factor. After the second QRG step, we are left with another square lattice with a lattice parameter equal to $3a$. The method preserves the ground state of the whole lattice when infinite cells are used. For our specific transformation cell, we find that the new renormalized sites have a constant energy value $G = E_-^{(1)}$. For the 2D isotropic AF Heisenberg, the two steps shown schematically in figure 1(*b*) yield $G^{(1)} = -4J - 4J' = -8J$, since $J' = J$ according to equation (3*b*). Following a well known method [10], the ground energy per spin is

$$E_{GS} = \sum_{l=1} G^{(l)}(J)/b^{dl} = \sum_{l=1} 8J^{(l)}/b^{dl}. \tag{5a}$$

From the above discussion, $J^{(l)} = J$ and our cell has the scaling factor $b = 3$ (see figure 1(*b*)). Thus

$$E_{GS} = (-8J/9)[1 + 1/9 + (1/9)^2 + \ldots] = -J. \tag{5b}$$

This result is 33% higher than the results of several methods as reviewed by Manousakis [11]. The same ground-state energy discrepancy for the Ising model with a transverse field is reported in [6], but, on the other hand, the QRG method gave a good quantitative description of its critical parameters. In fact, this method always yields an upper bound to the exact ground state owing to the truncation of the original Hilbert space. Therefore, such high ground-state energy is a consequence of the method; nevertheless, we expect that our QRG calculation gives a good qualitative description and an accurate phase diagram of the t–J model.

2.2. The recurrence relation for a single hole

In order to deal with the hole motion and to derive the QRG recurrence relation for one single hole on an AF background, we consider the following low-energy cell states (with $S = 0$):

$$|1, 0\rangle = (|+0-\rangle - |-0+\rangle)/\sqrt{2} \tag{6a}$$

$$|2, 0\rangle = (|+-0\rangle - |-+0\rangle + |0+-\rangle - |0-+\rangle)/2. \tag{6b}$$

These are the two lowest-energy states with one hole in a three-site cell and vanishing total spin. As before, we find the eigenvalues, keep the lowest one $E_-^{(0)}$ and its corresponding eigenvector (b_1, b_2) to define a renormalized hole state $|0'\rangle = b_1|1, 0\rangle + b_2|2, 0\rangle$. The

new cell operators are defined by the relations $C_+^{+\prime}|0'\rangle = |+'\rangle$ and $C_-^{+\prime}|0'\rangle = |-'\rangle$. The renormalized hopping amplitude is worked out in the same manner as J'. As shown schematically in figure 1(*a*), we calculate a matrix element, e.g. ${}_j\langle 0'|_i\langle +'|t'[C_{i+}^{+\prime}C_{j+}' + \text{HC}]|0'\rangle_i|+'\rangle_j$, with the intercell hopping term of the corresponding cells; this procedure yields

$$t' = \lambda^2(J, t)t \tag{7}$$

with

$$\lambda^2 = (b_2/2)^2[2a_1^2 + a_2^2 + a_3^2 - 2(a_1a_2 + a_1a_3)]. \tag{8}$$

We thus obtained the first part of the QRG for the hopping amplitude.

We again adopt the standard procedure [10] and define the renormalized chemical potential as the energy difference of the renormalized states. In general, there will be states with two or three holes that also become $|0'\rangle$ and states with one hole (like $|+0+\rangle$ that also become $|+'\rangle$). The average particle number for the $|+'\rangle$ state is 2.5 and 1.5 for the $|0'\rangle$ state. Thus the average chemical potential is

$$\mu' = 2(E_-^{(1)} - E_-^{(0)}). \tag{9}$$

Furthermore, we take $C' = E_-^{(0)}$ and the renormalized Hamiltonian has precisely the same form as the original one.

As a further test for our RG procedure, we applied the method to a 2D Hubbard model. We used the three-site cell states and energies of [10]. By similar arguments that led to the chemical potential, we obtain $U' = 2E^{\pm} - 2\mu + E^0$, where $E^{\pm}$ is the energy of the doubly occupied site. The hopping term, calculated by the above method, is twice the 1D hopping of [10] plus an additional term due to the hopping at the central site. After the two steps of figures 1(*a*) and (*b*), we obtain a non-trivial fixed point at $(U/t)_c = 4.98$. The detailed calculation, with critical exponent analysis, will be presented elsewhere. Such a value for the Mott transition compares better with the analytical calculations [12] than the value of 3.72 presented in [10].

2.3. The doped system with $t = 0$

We discuss now the doped system, which is an AF with vacant sites. The precise number of holes in the plane is dictated by the value of the chemical potential μ. Let us consider now the situation without the hopping term. This case corresponds to a quenched site diluted antiferromagnet with sites occupied either by electrons with probability p or by holes with probability $1 - p$. Clearly this probability depends on the degree of doping. Quenched site dilution is the case in which the configurational averages are independent of thermal averages and given by a separate site probability [13]. Since the original sites are occupied with probability p, then the renormalized cells may be defined to be occupied with probability p', and $p' = R(p)$. The function $R(p)$ depends only on the geometry of the chosen cell. In a general treatment using a majority rule, the states with two and three occupied sites with same z-component spin (like $|0++\rangle$, $|+0+\rangle$, ...) become the renormalized sites $|\pm'\rangle$. However, in order to use the results of the previous sections, we keep those with opposite spins (like $|0+-\rangle$, $|+0-\rangle$, ...) to become $|0'\rangle$. By the same

token, the states with two or three vacant sites should also become $|0'\rangle$. Based on these considerations, we can write the following general probability equations:

$$p' = p^3 + 3p^2(1-p)/2 \tag{10a}$$

$$1 - p' = 3p^2(1-p)/2 + 3(1-p)^2 p + (1-p)^3. \tag{10b}$$

Such equations do not have a finite fixed point and any finite concentration p flows to $p = 0$. The recurrence relation for the exchange coupling has to be modified to include the above dilution probability. Therefore we multiply both sides of equation (3*b*) by their respective site probability:

$$p'^2 J' = p^6 F(J) J/4. \tag{11}$$

The p'^2 comes from the two renormalized sites and the $p^6/4$ from the six sites of the two cells (figure 1(*a*)). This is the major correction near the half-filling where $p \simeq 1$. The factor of 4 is because only low-energy states that have total spin equal to 1/2, which are half of the total states, are considered in the calculations that led to equation (3*b*).

2.4. The doped system with hopping

Let us now consider the system described by the complete t–J Hamiltonian of equation (1). The motion of the electrons and holes introduces new features into the system: depending on whether it is more energetically favourable, the holes may either form a uniform-density phase through the whole plane or they may aggregate into two phases of different densities. These two possibilities are due to competition between the exchange coupling, which favours as many magnetic bonds as possible, and the hopping term, which favours the motion and, consequently, the separation of the spins. It is as if the hopping term plays the role of temperature in a dilute Heisenberg magnet at $T = 0$ K. When $t \neq 0$ (for $J \neq 0$) the system can phase-separate into hole-rich and electron-rich phases, exactly like the aggregation of a site diluted annealed magnetic system at low temperature. As the temperature is raised in an annealed magnet, several bonds are broken and and energetically unfavourable configurations may occur. On the other hand, this is the expected behaviour for a diluted magnet if the hopping amplitude t becomes of the order of J even at zero temperature.

In order to take these features into account, we introduce a zero-temperature 'annealed' site disorder, defined by an average over the two lowest-energy states for each cell:

$$\langle p \rangle = \frac{\exp[-(E_-^{(1)})/t] + 0 \times \exp[-(E_-^{(0)})/t]}{\exp[-(E_-^{(1)})/t] + \exp[-(E_-^{(0)})/t]} \tag{12a}$$

or

$$\langle p \rangle = \mathrm{e}^{-\mu'/t}/(\mathrm{e}^{-\mu'/t} + 1) \tag{12b}$$

where the exponents are divided by the hopping amplitude, t, just in order to be adimensional functions.

We want to generalize the QRG equations (4) and (7) for J' and t' derived for half-filling ($n \simeq 1$) in order to take the above mobile dilution into account. It is a strategy similar to what we did in equation (11): we take the probability of a renormalized electron $|+'\rangle$ or $|-'\rangle$ as $\langle p' \rangle$ and $\langle p^3 \rangle/2$ for the probability of the cell states used to calculate them. Similarly the probability of a renormalized hole $|0'\rangle$ is $(1 - \langle p' \rangle)$ and the cell states used to

calculate t' are $\langle p^3\rangle \times 3\langle p\rangle(1-\langle p\rangle)^2$. These probability weights provide a way to introduce the 'annealed' site disorder to our previous QRG equations. Thus the general QRG equations appropriate to the t–J Hamiltonian are

$$\langle p'\rangle^2 J' = \langle p\rangle^6 F(J) J/4 \tag{13a}$$

and

$$\langle p'\rangle(1-\langle p'\rangle)t' = 3\langle p\rangle(1-\langle p\rangle)^2\langle p\rangle^3\lambda^2(J,t)t. \tag{13b}$$

In order to obtain the complete recurrence relation, we note that J_H and t_H (see definition of J_H and t_H in figure 1(a)) are rescaled after the first step and become

$$\langle p'\rangle^2 J'_H = \langle p\rangle^6 J_H/4 \tag{14a}$$

and

$$\langle p'\rangle(1-\langle p'\rangle)t'_H = 3\langle p\rangle(1-\langle p\rangle)^2\langle p\rangle^3 t_H. \tag{14b}$$

We now perform the second step (figure 1(b)) and get the final QRG recurrence relation, which may be written as

$$\frac{\langle p'\rangle J'}{(1-\langle p'\rangle)t'} = \frac{F(J)\langle p\rangle^2 J}{12(1-\langle p\rangle)^2\lambda^2 t} \tag{15a}$$

and

$$\frac{\langle p''\rangle J''}{(1-\langle p''\rangle)t''} = \frac{\langle p'\rangle J'}{12(1-\langle p'\rangle)^2 t'} \tag{15b}$$

where we used $\lambda^2(J',t') = \lambda^2(J,t)$ in equation (15b), which is strictly true near the fixed points and therefore gives correct phase boundaries. Furthermore $\lambda^2(J,t)$ is a slowly varying function of J/t. On the other hand, we may rewrite equation (12b) as

$$\frac{\langle p\rangle}{1-\langle p\rangle} = \exp\left[2\left(\mu/t + 4J/t - \frac{3J/t + [(3J/t)^2+8]^{1/2}}{2}\right)\right]. \tag{16}$$

Therefore we arrive at complete QRG recurrence relations that recover the whole lattice and are dependent on the value of p, i.e. the electron concentration. In the large μ limit, n or $p = 1$ and we recover the results of the undiluted magnet (section 2.2).

3. Results

We present now the results of our QRG treatment. We consider the situation of isotropic spin coupling (Heisenberg model) and, just in order to gain insight on any out-of-plane interaction, the situation of anisotropic coupling (Ising model), the so-called t–J model [7].

For a given value of electron probability p (or electron density n), we analyse the recursion relation for J/t. In general we find an unstable (critical) fixed point $(J/t)_c$ and two trivial fixed points at $J/t = 0$ and $J/t = +\infty$. The value of the fixed point depends on the initial choice of electron probability p (or density n) and gives the phase boundary of

the zero-temperature t–J model phase diagram. For $J/t > (J/t)_c$ the RG iteration flow is towards the large J/t limit. For J/t below the critical value the flow is towards $J/t = 0$, which corresponds to a single uniform-density phase, with large kinetic energy holes.

We can demonstrate the phase separation by studying the recursion relation of equation (9) for the chemical potential in the Ising limit, which is

$$\mu' = 2\{\mu + 2J - [J + (J^2 + 8t^2)^{1/2}]/2\}. \tag{17}$$

For large J/t, $\mu' = 2(\mu + J)$. Near the half-filling situation, we start with $\mu_0 = 2J_0$, to get $\mu' = 6J_0$ after the first RG step. After the second step (see figure 1(*b*)), we obtain $\mu'' = 2(6J_0 + J') = 2(6J_0 + 3J_0) = 18J_0 = 9\mu_0 = b^d\mu_0$. Such an eigenvalue at a trivial fixed point equal to b^d is the signal for phase separation [14]. Although this calculation is performed for the Ising model, its conclusions can be extended to the Heisenberg model since the phase separation line is very similar and therefore both models yield the same phenomena. Thus we demonstrate here, for the first time, that the critical line separates a homogeneous-density from an inhomogeneous-density phase with a hole-rich and electron-rich phase and not a homogeneous antiferromagnetic from a homogeneous paramagnetic state.

The phase separation line is plotted in figure 2, for the Heisenberg case: the curve has a negative slope, indicating that the phase-separated state is first unstable to electrons appearing in the empty phase, as pointed out by Putikka *et al* [9]. The phase separation line starts near the value of $n = 0.89$ and $J/t = 0$. It is important to verify that we find a change of phase at $n \simeq 0.8$ and $J/t \simeq 0.3$, which are values close to the experimental observations for some HTSC compounds. The critical line finishes at $J/t \simeq 1.9$ for $n = 0$. The Ising separation line is very close to the Heisenberg line.

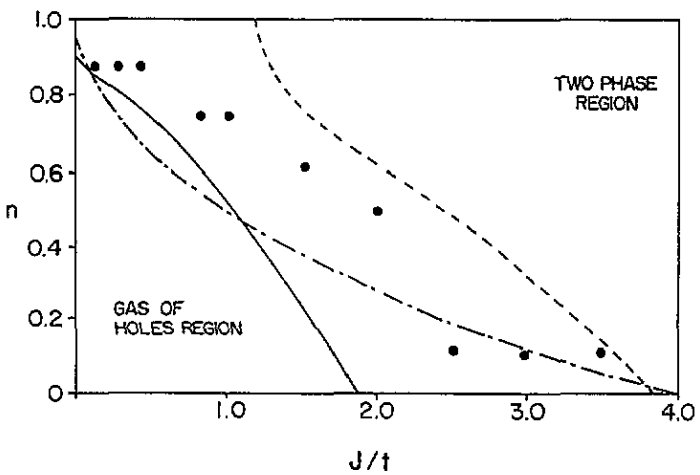

Figure 2. The results of our calculations. We include the curve of [8] (- - - -) and the curve of [9] (— · —). The points are the results of [7].

We also display in figure 2 some previous results for the 2D t–J model phase diagram. The calculations of Marder *et al* [8] compare better with our results for low J/t but are closer to the Ising model calculations. This may be a consequence of their semiclassical theory and the modification of the Hubbard operators commutation relations. The results

of Emery *et al* [7] agree with our results for $n \simeq 0.7$ and also display phase separation for very low values of J/t. They have performed an exact numerical diagonalization on a 4×4 cluster and used the general arguments of [15] and [16]. Nevertheless, it is not straightforward how their results are extended to the infinite square lattice. Also plotted in figure 2 are the calculations of Putikka *et al* [9]. They have performed a high-temperature expansion for the Helmholtz free energy and used Padé and integral approximants to estimate the $T = 0$ K behaviour. They found that phase separation may occur only for $J/t > 1.2$, which is significantly different from all the other calculations and is against some theoretical arguments [15, 16], which favour phase separation also in the limit of small J/t.

Our line starts at $n = 1.0$ and $J/t = 0$ and stays near this value of J/t down to $n = 0.9$ where J/t grows very rapidly. The small values of J/t for the transition line may be attributed to the large fluctuation of the density in a small cell. In other words the value of p flows very quickly to $p = 0$. This also explains how our calculation falls much faster than in [7], [8] and [9] in the dilute regime. Furthermore we used states near the half-filling to calculate the scaling parameters $F(J)$ and $\lambda(J, t)$. Thus our results are more accurate in the regime above $p = 0.5$, where it is more interesting in order to compare with HTSC.

4. Conclusions

We have performed a real-space QRG analysis of the zero-temperature phase diagram of the 2D t–J model. This technique has been used successfully for several different quantum systems [6], and yields good quantitative results for the low-energy and low-temperature properties.

The method gives the expected zero-temperature recurrence relation for the Ising and Heisenberg coupling constant. We also applied the method to the 2D Hubbard model and obtained a Mott transition in better agreement with analytical calculations [11] than previous RG calculations [10]. These tests and the partial agreement with the exact diagonalization of a 4×4 cluster [7] give us confidence in our procedure.

A critical line is found that separates two distinct regions: one of a gas of holes in an antiferromagnetic background and another consisting of a phase in which holes segregate in a hole-rich and a pure antiferromagnetic region. We were able to demonstrate the phase separation applying some well known renormalization-group results [14] to the chemical-potential recurrence relation near the phase attractor. It ruled out the possibility of some magnetic reordering change of phase. We thus conclude that the QRG technique may be used to calculate the phase frontiers and also to characterize the phases.

The phase separation line agrees extremely well with the known values of the doping concentration and spin coupling for lanthanum HTSC, indicating that the t–J model, despite its simplicity, may describe the essential physics of HTSC.

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