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Studies of the spin diffusion coefficient and the spin stiffness constant for the t–J model on low-dimensional lattices and possible application to doped antiferromagnets

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Abstract

The spin response functions for a doped strongly correlated quantum Heisenberg antiferromagnet, in the form of a t–J model, on low-dimensional lattices have been explored. In particular, the spin stiffness constant and the spin diffusion coefficient have been calculated as functions of doping concentration by different approaches for this model on a chain and on a square lattice. The occurrences of various possible magnetic phases, namely with long range and short range orders, and also a novel paramagnetic phase, have been predicted at zero temperature. Our conclusions regarding the phase diagram agree remarkably well with those from other recent theoretical approaches. Our results are discussed in the light of experimental results from the cuprates.

1. Introduction

The microscopic mechanism behind the occurrence of high temperature superconductivity in the cuprates is still controversial [1]. Nevertheless many of these compounds are products of doping of parent insulating antiferromagnetic systems. Thus it is quite likely that the analysis of the state of a doped, strongly correlated insulator displaying quantum antiferromagnetism will be useful for understanding the anomalous normal phase and the possible mechanism for high temperature superconductivity. Moreover, the effect of doping on the long range antiferromagnetic ordering is itself an interesting and challenging problem in theoretical condensed matter physics [2, 3].

In this paper, we investigate the magnetic correlations for a doped quantum antiferromagnet in two dimensions in the form of a strongly correlated t–J model involving holes, at zero temperature. This model is especially important in view of the discovery of high temperature superconductivity in layered cuprate systems. Besides the spin response, the charge response functions are equally important for this model, as the cuprates show a very rich phase diagram exhibiting antiferromagnetism, paramagnetism, pseudo-gap, stripes with

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phase separation and, of course, superconductivity, at various levels of hole concentration [4]. However, the t–J model is too simple and may not be able to capture all the important physics of the cuprates. It is believed that the t–J model is most suitable to investigate the magnetic properties of a doped quantum antiferromagnet, particularly in the underdoped regime. It is in this spirit that we have taken up the present study. Nevertheless, it may be important to study the charge response of this model as well, using our formalism in the near future to verify the predictions regarding possible 'phase separation' and the electronic charge transport obtained from various numerical and approximate analytical calculations [5, 6]. It would be interesting in particular to calculate the charge stiffness constant and examine the possibility of its softening leading to a phase separation.

Regarding the spin response, there have been several theoretical attempts involving both analytical and numerical techniques [2, 3, 7, 8]. The conclusions, however, were varied. This is partly also because of the finer differences in the description of this model itself. Besides, in most of these calculations the evolution of antiferromagnetism with hole doping was not predicted and analysed in detail. On the contrary, in many cases the mathematical form of the weakening of antiferromagnetism with doping was assumed or incorporated phenomenologically. Therefore it remains quite challenging to examine how far the t–J model can successfully make predictions regarding the magnetic phase diagram of low-dimensional doped quantum antiferromagnets.

The physical quantities we calculate here are the spin diffusion coefficient and the spin stiffness constant as functions of the doping concentration. By combining and analysing our calculational results, we sketch out the corresponding phases, as the hole concentration is varied starting from the half-filled band limit. The results indeed exhibit the weakening of antiferromagnetism with doping and the quantum melting of the spin system after a critical doping concentration, in very good quantitative agreement with some of the recent theoretical approaches and qualitatively with the experimental results from cuprates [2–4]. In particular, we demarcate the regime of the finite order parameter (true long range order), the one with decaying correlations and the completely uncorrelated paramagnetic regime, all appearing at zero temperature in our calculations. Moreover, we also argue that the paramagnetic regime obtained in our calculations is of non-conventional type.

2. Model and mathematical formulation

The Hamiltonian of the strongly correlated t–J model is given by [7]:

$$\mathcal{H}_{t-J} = \mathcal{H}_t + \mathcal{H}_J, \tag{1}$$

where

$$\mathcal{H}_t = \sum_{ij\sigma} t_{ij} X_i^{\sigma 0} X_j^{0\sigma} \tag{2}$$

and

$$\mathcal{H}_J = \sum_{ij} J_{ij} (\mathbf{S}_i \cdot \mathbf{S}_j - (1/4) n_i n_j), \tag{3}$$

where Xs are the Hubbard operators, and the spin operators can be expressed in terms of the Hubbard operators as [7]:

$$\hat{\mathbf{S}}_i^+ = X_i^{\sigma 0} X_i^{0\bar{\sigma}}, \qquad \hat{\mathbf{S}}_i^- = X_i^{\bar{\sigma} 0} X_i^{0\sigma}, \qquad \hat{\mathbf{S}}_i^z = (1/2) \sum_\sigma \sigma X_i^{\sigma\sigma}. \tag{4}$$

Besides, we also have for the number operator,

$$\hat{n}_i = \sum_\sigma X_i^{\sigma\sigma}. \tag{5}$$

Because of the presence of strong correlation, only singly occupied sites are retained in the t–J model and the completeness relation for the Hubbard operators is [7]:

$$X_i^{00} + \sum_\sigma X_i^{\sigma\sigma} = 1. \tag{6}$$

We now define the two principal quantities of interest, namely the spin diffusion coefficient and the spin stiffness constant.

The spin diffusion coefficient is given by the expression [7],

$$D^{\mathrm{sd}} = \frac{D}{\chi_0}, \tag{7}$$

where

$$D = D_t + D_J, \tag{8}$$

where D_t represents the hopping contribution and D_J represents the exchange contribution to the total dc spin conductivity D; χ_0 is the static uniform spin susceptibility. In our case, D includes the effect of spin dynamics explicitly and completely besides the usual contributions from transport.

The spin stiffness constant $\mathcal{D}_{\mathrm{spin}}$ is defined as [9],

$$\mathcal{D}_{\mathrm{spin}} = \lim_{\Phi\to 0}\left(\frac{1}{2}\right)\frac{\delta^2 E}{\delta\Phi^2}, \tag{9}$$

where $E(\Phi)$ is the total ground state energy in the presence of the staggered Peierl's phase (resembling a magnetic flux) Φ_σ, arising from an applied vector potential $\mathbf{A}(\mathbf{r})$, such that

$$\Phi_\downarrow = -\Phi_\uparrow = \Phi. \tag{10}$$

Moreover, in the presence of this staggered phase the hopping amplitude t_{ij} for a fermion with spin σ is modified to $t_{ij}\mathrm{e}^{\mathrm{i}\Phi_\sigma}$, provided the vector potential has a component along the direction of hopping.

The significance of the studies in D and $\mathcal{D}_{\mathrm{spin}}$ is that these quantities can detect the presence of the long range magnetic order and the existence of spin–spin correlations in the system. To be more precise, D provides information regarding the damping of the collective spin excitations whereas $\mathcal{D}_{\mathrm{spin}}$ measures an effective antiferromagnetic exchange coupling, as we will see in detail in the next section.

3. Calculations and results

We start from the formal expressions for D_t and D_J obtained in our earlier work for the strongly correlated t–J model in 2D [7].

$$D_t = \frac{\pi}{N}\sum_{\mathbf{k}}(\hat{\mathbf{q}}\nabla_{\mathbf{k}}t_{\mathbf{k}})^2 \lim_{\omega\to 0}\lim_{\mathbf{q}\to 0}\int_{-\infty}^{\infty} \mathrm{d}\omega_1 |n'(\omega_1)| \mathcal{A}_{\mathbf{k}}(\omega_1)\mathcal{A}_{\mathbf{k}-\mathbf{q}}(\omega_1-\omega), \tag{11}$$

where $\mathcal{A}$ denotes the single hole spectral function corresponding to the coherent part of the single hole Green's function and $t_{\mathbf{k}}$ is the Fourier component of the hopping integral. As is well known, the spectral function for one-hole excitations in this model can be written as a sum of the coherent part arising from the quasi-particle propagation in a narrow band of the order of $2J$ and an incoherent part due to diffusive motion of holes in a broad band of bandwidth $4t$ [9].

This expression takes the following form in the doped phase, after simplification:

$$D_t(n) = \sum_{\mathbf{k}} C_{\mathbf{k}}^2\Bigg[-\frac{(1+n)^2}{4}[\delta(r-\epsilon_{\mathbf{k}})]^2 - N_{\mathrm{inc}}\theta(W-|r|)[(1+n)\delta(r-\epsilon_{\mathbf{k}}) + N_{\mathrm{inc}}\theta(W-|r|)]\Bigg], \tag{12}$$

where $D_t(n)$ is the doping dependent contribution to the spin conductivity from hopping, $C_{\mathbf{k}}^2$ stands for $\frac{\pi}{N}(\hat{\mathbf{q}}\nabla_{\mathbf{k}}t_{\mathbf{k}})^2$, $N_{\rm inc}$ denotes the density of states corresponding to the incoherent part of the single hole Green's function, n is the original carrier (hole) concentration ($n = 1$ is the half-filled limit) and r is given by:

$$r = \frac{2W(1-3\delta)}{1+\delta} \tag{13}$$

with W as the bandwidth corresponding to the incoherent part of the hole motion and $\delta = 1 - n$ is the doping level (concentration of vacancies). In order that the true long range antiferromagnetic order exists at zero temperature, we must have the doping dependent spin conductivity $D(n) = D_t(n) + D_J(n)$ vanishing. This criterion is based on the fact that the collective excitations for a quantum spin system with long range ordering should be undamped as temperature approaches zero [10]. One way of achieving that is to have both $D_t(n)$ and $D_J(n)$, determined self-consistently, to vanish separately. The condition for $D_t(n)$ to vanish can be expressed as:

$$2W(1-3\delta)/(1+\delta) \geqslant W \tag{14}$$

leading to

$$\delta \leqslant 1/7. \tag{15}$$

This also ensures that $\epsilon_{\mathbf{k}}$ is not equal to $2W(1-3\delta)/(1+\delta)$ and as a result all terms in the above equation for $D_t(n)$ vanish. This condition is consistent with the constraint that $\epsilon_{\mathbf{k}}$ is less than 2μ for all k where μ is the chemical potential. This inequality is expected to hold for an underdoped Mott–Hubbard system [8]. Thus we may conclude that $D_t(n)$ vanishes, as long as the doping concentration does not exceed 0.14.

Again $D_J(n)$, the exchange contribution to spin conductivity in the doped case is given by [7, 8]:

$$D_J(n) = \lim_{\omega\to 0}\lim_{\mathbf{q}\to 0}\int_{-\infty}^{\infty} {\rm d}\omega_1 |N'(\omega_1)| {\rm Im}\,\chi_{\mathbf{k}}(\omega_1) {\rm Im}\,\chi_{\mathbf{k}-\mathbf{q}}(\omega_1-\omega), \tag{16}$$

where

$$\chi_{\mathbf{q}}(\omega) = \chi_0 i D^{\rm sd}q^2/(\omega + {\rm i}D^{\rm sd}q^2), \qquad N'(\omega) = {\rm d}N(\omega)/{\rm d}\omega, \qquad D^{\rm sd} = D/\chi_0. \tag{17}$$

The quantity $N(\omega)$ is the Bose distribution function and the quantity $\chi_{\mathbf{q}}(\omega)$ is the wavevector dependent dynamical spin susceptibility. We now analyse the quantity $N'(\omega)$.

$$N(\omega) = 1/({\rm e}^{\beta\omega} - 1). \tag{18}$$

Thus as T approaches zero, $|N'(\omega)|$ can be shown to behave like $\delta(\omega)$. Therefore from the equation written earlier for $D_J(n)$, we see that $D_J(n)$ itself vanishes at zero temperature. This is quite similar to the result as expected for a pure Heisenberg spin model. Thus only $D_t(n)$ contributes. Therefore the total spin diffusion coefficient remains zero for $\delta \leqslant 0.14$ at zero temperature, as χ_0 is expected to be finite [8]. So for doping concentration below 0.14, the long range antiferromagnetic order is stable at zero temperature. This implies that there exists a non-zero value of the Néel temperature $T_{\rm N}$ (if the system is made quasi-two-dimensional) as long as the doping level is less than 14%. This magnitude of critical doping concentration is very close to the corresponding threshold value of about 12% obtained by Himeda and Ogata [2] in an improved variational calculation. The interesting aspect of our result is that this threshold value of doping is independent of J, although $T_{\rm N}$ itself depends on J as well as on the hole concentration.

Let us now focus our attention on the higher doping regime where the long range antiferromagnetic order is absent. We take up the calculation of the spin stiffness constant

for the strongly correlated t–J model as a function of doping concentration. The objective is to study the evolution (renormalization) of the antiferromagnetic exchange constant J itself with doping, which was not addressed at all in the calculation for D. For simplicity, we consider both the hopping term and the exchange term in the nearest neighbour approximation.

The total spin stiffness constant $\mathcal{D}_s$ may be written as:

$$\mathcal{D}_s = \mathcal{D}_s^t + \mathcal{D}_s^J, \tag{19}$$

where $\mathcal{D}_s^t$ and $\mathcal{D}_s^J$ are the contributions from the t term and the J term respectively.

$$\mathcal{D}_s^t = \lim_{\Phi\to 0}\left(\frac{1}{2}\right)\left(\frac{\delta^2 T}{\delta\Phi^2}\right) \tag{20}$$

and

$$\mathcal{D}_s^J = \lim_{\Phi\to 0}\left(\frac{1}{2}\right)\left(\frac{\delta^2 E_J{}^{sf}}{\delta\Phi^2}\right), \tag{21}$$

where T is the kinetic energy contribution and E_J^{sf} is the spin flip part of the exchange energy contribution (E_J) to the total energy of the ground state. From the very definitions, E, T and E_J are the expectation values of $\mathcal{H}_{t-J}$, $\mathcal{H}_t$ and $\mathcal{H}_J$ respectively in the ground state. It follows from our calculations, to be elaborated later, that the direct part of the exchange energy term does not contribute to $\mathcal{D}_s^J$. The quantity Φ denotes the magnitude of the staggered phase, as mentioned before.

From these defining equations it can be seen that $\mathcal{D}_s$ per site may be regarded as a quantity proportional to an 'effective antiferromagnetic exchange constant J_{eff}', as it measures the kinetic correlation between the holes with up spin and down spin. Again J_{eff} may be looked upon as a bare antiferromagnetic exchange constant J, seen in the undoped phase, renormalized by the sea of mobile holes in the doped phase. Thus when $\mathcal{D}_s$ vanishes, the antiferromagnetic correlations also vanish—leading to the destruction of even short range antiferromagnetic order.

In calculating E, the ground state energy, we adopt a simplified procedure. To avoid the complicated and messy calculation involving Hubbard operators, we evaluate E using a very well known and widely used form for the strongly correlated ground state, namely the Gutzwiller state containing the usual fermion operators, with the 'no double occupancy condition' (NDOC) imposed directly on it. However, it must be remarked that the results are not expected to be very sensitive to the choice of the form of the trial state. The very general form of the Gutzwiller state is given by:

$$|\psi_G\rangle = \prod_1\prod_{\mathbf{k},\sigma}\sum_{i,j}(1-\alpha\hat{n}_{l\uparrow}\hat{n}_{l\downarrow})c_{i\sigma}^{+}c_{j-\sigma}^{+}e^{i(\mathbf{r}_i-\mathbf{r}_j)\cdot\mathbf{k}}|\text{vac}\rangle, \tag{22}$$

where $|\text{vac}\rangle$ is the vacuum state (having fermionic occupation number equal to zero) and we have omitted the normalization constant for the time being. The symbols i, j and l denote the lattice sites and $\mathbf{k}$ represents the wavevector for the fermion, in this case the existing hole. The magnitude of $\mathbf{k}$ is bounded by k_F (Fermi wavevector) from above. The variational parameter α is determined by minimizing the expression for E; whereas E is the expectation value of $\mathcal{H}_{t-J}$ in the Gutzwiller state itself. Here, however, as we would like to incorporate the effect of Hubbard operators occurring in $\mathcal{H}_{t-J}$, not allowing the double occupation of a site by fermions at all in this doped antiferromagnetic phase, we must incorporate $\alpha = 1$ in the present case and then determine the actual E. Moreover, for this calculation, only fermion operators are used in $\mathcal{H}_{t-J}$. This is totally consistent with the strong correlation assumed to be present in the lightly doped phase of the quantum antiferromagnet, as described by the t–J model containing the Hubbard operators. This Gutzwiller state vector, with the variational parameter set equal to 1

implying a Fermi sea with the doubly occupied sites completely projected out, is given by [11]:

$$|\psi_{\rm G}\rangle_{\rm NDOC} = \prod_{1}\prod_{\mathbf{k},\sigma}\sum_{i,j}(1-\hat{n}_{l\uparrow}\hat{n}_{l\downarrow})c^{+}_{i\sigma}c^{+}_{j-\sigma}{\rm e}^{{\rm i}(\mathbf{r}_i-\mathbf{r}_j)\cdot\mathbf{k}}|{\rm vac}\rangle. \tag{23}$$

We take this quantum state $|\psi_{\rm G}\rangle_{\rm NDOC}$ as our ground state for carrying out calculations of the expectation values.

Then, the kinetic energy contribution of the fermionic system in the presence of the staggered phase Φ_σ is given as (by incorporating the phase Φ in the modified $t_{i,j}$ in $\mathcal{H}_{t-J}$):

$$T(\Phi\neq 0) = 2\prod_{l,l'(nn)}\prod_{\mathbf{k},\mathbf{k}',\sigma}[\sum_{ij\sigma}\cos(\Phi_\sigma/L-(\mathbf{r}_i-\mathbf{r}_j)\cdot(\mathbf{k}-\mathbf{k}')) - \cos(\Phi_\sigma/L-(\mathbf{r}_{l'}-\mathbf{r}_{\rm l})\cdot\mathbf{k}')]t, \tag{24}$$

where we will have to use equation (10) for Φ_σ corresponding to up spin and down spin respectively, t is the magnitude of t_{ij} with ij as nearest neighbours, L is the length of the box and i, j, l, l' are the lattice sites. In deriving equation (24), we have made use of the usual fermionic algebra and also the orthogonality of $|{\rm vac}\rangle$ with any quantum state having finite fermionic occupation number. $T(\Phi=0)$ can easily be obtained from equation (24) by substituting $\Phi=0$. Next we will have to evaluate $E_J(\Phi)$. This can easily be done provided we assume a relation between J and the effective hopping amplitude. Without getting into the details of various proposed microscopic derivations of the generalized t–J model we, for simplicity, model J as $2t^2_{\rm eff}/V_{\rm eff}$ where $t_{\rm eff}$ is the effective nearest neighbour hopping amplitude and $V_{\rm eff}$ is the effective barrier potential encountered in the hopping, within the effective one-band scenario [8]. It is worthwhile mentioning that t and $t_{\rm eff}$ are in general different; however, we have assumed both of them to be real for simplicity. Moreover, both obey the same transformation law in the presence of the vector potential. In the calculation for the expectation value of $\mathcal{H}_J(\Phi)$ in the state $|\psi_{\rm G}\rangle_{\rm NDOC}$, we notice a few features. First of all, only when the two near neighbour sites are occupied (singly occupied) is there a finite contribution, otherwise not. Secondly, since the phase is staggered (see equation (10)), it can be seen easily that only the spin flip terms will retain a Φ-dependence in the super-exchange process. In the non-spin flip terms the Φ-dependence will be absent. Then the result comes out to be:

$$E^{\rm sf}_J(\Phi) = ((4t^2_{\rm eff}\cos(2\Phi))/V_{\rm eff})\langle\psi_{\rm G}|_{\rm NDOC}\mathcal{H}^{\rm sf}_J|\psi_{\rm G}\rangle_{\rm NDOC}, \tag{25}$$

where $\mathcal{H}^{\rm sf}_J$ is the spin flip part of the exchange interaction term. The above expectation value can now be evaluated by locating the nearest neighbour positions for both a one-dimensional chain and a two-dimensional square lattice. Carrying out the calculation by expressing all the spin operators for a spin $\frac{1}{2}$ particle in terms of the fermion operators in the standard way (we need not involve Hubbard operators as we are already working with $|\psi_{\rm G}\rangle_{\rm NDOC}$) and after performing the standard but detailed algebra, we find that both for a one-dimensional chain and a two-dimensional square lattice with nearest neighbour spin–spin coupling the following equation is obtained:

$$\langle\psi_{\rm G}|_{\rm NDOC}\mathcal{H}^{\rm sf}_J|\psi_{\rm G}\rangle_{\rm NDOC} = JN_{\rm l}, \tag{26}$$

where $N_{\rm l}$ is the expectation value of the number operator corresponding to the total number of lattice sites singly occupied by spins. This equation (26) is intuitively expected! Again by the very definition, $N_{\rm l}$ is obviously a doping dependent quantity. More precisely,

$$N_{\rm l} = N(1-\delta), \tag{27}$$

where δ is the doping (vacancy) concentration and N is the total number of sites in the lattice, occupied or unoccupied by spins. Thus from the equations (21), (25) and (26), we have

$$\mathcal{D}^J_{\rm s} = -4JN_{\rm l}. \tag{28}$$

Therefore the critical value of δ at which the antiferromagnetic correlations vanish completely is obtainable from the equation:

$$\mathcal{D}_{\rm s}^{t} + \mathcal{D}_{\rm s}^{J} = 0. \tag{29}$$

This equation includes the contributions from both dynamical effects and the dilutional effects arising from the presence of the vacancies.

Now we can analyse various cases, namely situations in one dimension (1D) and two dimensions (2D). Let us first look at the situation in 1D. For simplicity, we neglect the band structure effects. We take the continuum approximation and consider a hole Fermi sea. Making use of the equations (20) and (24) and after a long calculation involving the evaluation of the derivatives with respect to Φ, twice of the product of cosine functions and the combination of the terms properly, we arrive at the following equation:

$$\mathcal{D}_{\rm s}^{t} = (-t)\prod_{l,l'}^{L}\prod_{k,k'}^{k_{\rm F}}\left[\sum_{\langle ij\rangle} 2\cos((r_i - r_j)\cdot(k - k')) - 2\cos(k'a)\right], \tag{30}$$

where $k_{\rm F}$ is the Fermi wavevector corresponding to the 'hole Fermi sea' (related to the surviving holes) and a is the lattice spacing. It should be emphasized, however, that this 'hole Fermi sea' is just one of the mathematical components of the $|\psi_{\rm G}\rangle_{\rm NDOC}$ state, representative of the actual quantum state of the holes (see equation (23)). Now as we can see, $\mathcal{D}_{\rm s}^{t}$ becomes a function of doping concentration δ through the appearance of $k_{\rm F}$ in the expression. Therefore the only task remaining is to examine whether an allowed solution for δ exists to satisfy the vanishing of $\mathcal{D}_{\rm s}$. It can easily be seen that if we demand $\mathcal{D}_{\rm s}$ to be zero, then we get a consistent solution only when both $\mathcal{D}_{\rm s}^{t}$ and $\mathcal{D}_{\rm s}^{J}$ are simultaneously zero, as the parameters t and J are independent in this model. The conditions for the vanishing of $\mathcal{D}_{\rm s}^{t}$ are the following: (i) at least one point in the k' space should satisfy

$$k'a = (2m + 1)\pi/2 \tag{31}$$

or (ii) the difference δk between two points in the k (or k' space) should obey

$$\Delta k = (2p + 1)\pi/2, \tag{32}$$

where m and p are any integers and $|k'|$ (and $|k|$ too) is bounded between zero and $k_{\rm F}$. Again from the k-space density of states we easily get,

$$k_{\rm F} = (\pi/2a)n, \qquad n = N_{\rm f}/N, \tag{33}$$

where $N_{\rm f}$ is the total number of fermions (holes) in a chain containing N sites.

Thus for n tending to 1, i.e. for δ tending to zero, we can satisfy the constraints on the k (or k') space, for making $\mathcal{D}_{\rm s}^{t}$ vanish. Besides, for n equal to $\frac{1}{2}$, i.e. corresponding to δ equal to 0.5, the constraints can again be satisfied to make $\mathcal{D}_{\rm s}^{t}$ vanish. There is one more possibility for $\mathcal{D}_{\rm s}^{t}$ to go to zero, however. This can be achieved by making $k_{\rm F}$ vanishingly small, corresponding to the limit δ tending to 1. It can be seen very easily from our earlier expression that only for δ equal to 1, does $\mathcal{D}_{\rm s}^{J}$ also vanish. Thus we can say that in 1D the antiferromagnetic correlations can be completely killed only when the doping level reaches 100%. This reminds one of the similar result obtained in the case of the 1D Hubbard Model [9]. It is worthwhile mentioning that the results for the 1D t–J model studied by the various other exact methods have all been obtained for some special ratios of the parameters t and J [9].

Now, let us analyse the situation in 2D, which is of chief interest to us. As usual, the vector potential field $A(\mathbf{r})$ is assumed to have been applied along the **x** direction. We again carry out the calculation in the continuum approximation, exactly in the same way as in 1D.

$$\mathcal{D}_{\rm s}^{t} = (-t)\prod_{\mathbf{l},\mathbf{l}'}\prod_{\mathbf{k},\mathbf{k}'}^{k_{\rm F}}\left[\sum_{\langle ij\rangle} 2\cos((r_i^x - r_j^x)\cdot(k_x - k_x')) - 2\cos(k_x'a)\right]. \tag{34}$$

The conditions for the vanishing of $\mathcal{D}_s^t$ are very similar to the ones found in 1D. As before, one condition is that at least one k'_x value (from the whole set) should obey the following:

$$k'_x = (2m+1)\pi/2a, \qquad (k'_x)_{\min} = \pi/2a. \tag{35}$$

We also have,

$$((k_x^{\max})^2 + (k_y^{\max})^2)^{1/2} = k_F, \qquad k_F = (2\pi N_f)^{1/2}/(N-1)a, \qquad k_F^2 = \frac{2\pi(1-\delta)}{a^2}. \tag{36}$$

Now to satisfy the vanishing of $\mathcal{D}_s^t$, we must have

$$(k_F)_{\text{threshold}} = \pi/2a. \tag{37}$$

This leads to

$$n \geqslant 0.39, \tag{38}$$

where n represents the original carrier (hole) concentration. Thus for doping concentrations of 0.61 or less, $\mathcal{D}_s^t$ becomes zero. The other condition, namely $\Delta k'_x = \pi/2a$, again leads to a doping concentration of 0.5 or less for spin stiffness due to hopping to vanish. For field applied along the y-direction too we get the same result. For field applied along any general direction, one can easily show that for $\mathcal{D}_s^t$ to vanish we need,

$$(k'_x + k'_y)_{\min} = \pi/2a. \tag{39}$$

We also have,

$$k_F^2 \geqslant ((k'_x)^2 + (k'_y)^2)_{\min}. \tag{40}$$

This reduces to

$$n \geqslant \pi/16. \tag{41}$$

Thus for doping concentrations of about 80% or less, $\mathcal{D}_s^t$ vanishes. The other condition involving $\Delta\mathbf{k}$ is more difficult to satisfy in this case. Nevertheless, in all the three cases mentioned above there is one common condition, namely k_F tending to zero (occurring at $\delta = 1.0$), which also leads to the vanishing of the spin stiffness arising from the hopping. Thus in the limit of infinitesimal J, the regime of non-zero $\mathcal{D}_s^t$ above $\delta = 0.14$, represents the short range ordered state. Therefore, in general, this short range spin correlation, driven entirely by the restricted hopping in this case, persists between doping concentration of 0.61 to just below 1.00. We believe this is a new result, as this case with infinitesimal J has not been investigated in detail in the context of the t–J model.

Let us now examine the other situation, namely that of finite J. Here as seen earlier in 1D, the only allowed solution for the total spin stiffness to vanish is $\delta = 1.0$. Thus for finite J, the short range spin correlations having contributions from both the restricted hopping term and the exchange term persist in the regime $0.14 \leqslant \delta < 1.0$. This result is in quantitative agreement with the prediction of Himeda and Ogata [2] that the antiferromagnetic correlations survive up to the doping level approaching 100%.

4. Conclusions

From our detailed calculations for spin responses presented in the last section, we see that for doping concentrations between 0.14 and 0.61 the spin stiffness constant corresponding to the 2D t–J model goes to zero in the case of an infinitesimal value of J. This leads to complete destruction of antiferromagnetic correlations in this doping regime. It is interesting to note that the non-zero value of the spin stiffness, present in the doping regime outside the

Table 1. Magnetic phases as a function of doping for infinitesimal J.

δ	Phase
$0 \leqslant \delta < 0.14$	Long range ordered
$0.14 \leqslant \delta < 0.61$	Novel paramagnetic
$0.61 \leqslant \delta < 1.0$	Short range ordered

Table 2. Same as table 1 but for finite J.

δ	Phase
$0 \leqslant \delta < 0.14$	Long range ordered
$0.14 \leqslant \delta < 1.0$	Short range ordered

above range, corresponds to an 'effective spin–spin correlation' between the mobile holes—arising almost entirely from their constrained hopping, as J tends to zero here. This scenario further predicts holes with completely uncorrelated spins in this regime $0.14 \leqslant \delta < 0.61$, signifying a truly paramagnetic phase of the mobile holes. This, however, is different from the usual itinerant paramagnetism, seen in Fermi liquids, on two accounts. Firstly, NDOC at each site will still have to be strictly obeyed. Secondly, the correlation between the up and the down spins in the hopping process is absent completely. However, at higher doping concentrations, the correlations between holes with anti-parallel spins ($\mathcal{D}_s$) reappear. This now leads to a paramagnetic phase with short range ordering, again distinct from the Fermi liquid-like paramagnetic state because of NDOC. This new phase persists up to doping concentrations just below 100%.

In the other situation, namely with finite value of J, the spin stiffness constant remains non-zero for the entire doping range below 1.0. Earlier, from our calculation of the spin diffusion constant, well defined undamped long wavelength spin excitations were found to exist for doping levels up to 14%, implying that the long range antiferromagnetic order persists up to that doping level for finite value of J. These two limits are very significant. One possible scenario emerging from this is that the 'true long range' AF order persists up to δ equal to 0.14 and thereafter in the intermediate regime of δ lying in the range from 0.14 to just below 1.0, we again have the 'antiferromagnetically correlated' paramagnetic phase. The nature of this phase with short range order appears to be quite complex and will be investigated soon. This analysis also implies that any serious theoretical attempt to explore superconductivity within the framework of the t–J model must take into consideration these persistent antiferromagnetic correlations [6]. Our conclusions regarding the magnetic phase diagram are summarized in tables 1 and 2. In general, however, there will be a parallel phase diagram for charge response which coexists with the spin response diagram.

Our results in the regime of vanishingly small J, bear a similarity to the 'spin polaron' scenario [12] within the non-Fermi liquid framework. In the other situation, namely J having finite magnitude, the scenario of correlation between 'local moments' [13] seems to be a more relevant description from our analysis. These results look qualitatively similar to the ones obtained by SchmittRink *et al* [14] in the context of the dynamics of one hole in the background of an antiferromagnet within the purview of a t–J-like model. It may also be interesting to comment on a few other approaches [15] for calculations of the spin diffusion coefficient of the t–J model. Our approach is distinct from that of Meisner *et al* [15] as our spin current density operator takes care of both hopping (transport) and exchange interaction processes explicitly in the calculation for D [7]. On the other hand the work of Bonca and Jaklic [15] neglects the

spin flip processes and its semi-analytical–semi-numerical approach handles only very specific parameter ratios outside the high-T_c regime.

Before concluding, let us make a few more remarks. The t–J model is strictly valid only in the low-doping regime. Therefore the critical values of the doping concentration corresponding to the phase boundaries, as obtained in our calculations, may not always have quantitative agreement with the corresponding experimentally observed ones for the two-dimensional and quasi-two-dimensional doped antiferromagnets at very low temperatures. Besides, in our calculations we have neglected the band structure effects completely. In addition, the inter-layer processes, which are believed to play very important roles in determining the phase boundaries in some of the cuprates, have not been considered at all in our calculations for pure 1D and 2D systems. Nevertheless, our approach does bring out the existence of some distinct magnetic phases with interesting properties from the t–J model on the low-dimensional lattices. Furthermore, this has quantitative support from some of the other recent theoretical approaches and broad qualitative support from the experimental results for the magnetic properties of some of the cuprates [2–4, 16].

Our future plans includes the investigation of the charge response and exploration of the possible microscopic phase separation processes for this model, by making use of the same formalism as has been employed here. This would enable us to have a complete phase diagram for this model.

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