Investigation of the magnetic behaviour of doped quantum antiferromagnets on low-dimensional lattices

Suraka Bhattacharjee

S.N. Bose National Centre for Basic Sciences, Kolkata, India

Email: surakabhatta@bose.res.in

Highlights

➢ ***The interesting magnetic behaviour of the low-dimensional strongly-correlated under-doped quantum antiferroamgnets is manifested in their unusual properties.***

➢ ***I have used the strongly correlated t-J model as the basis for the derivation of generalized spin stiffness constant for these doped systems in one and two dimension.***

➢ ***The magnetic behaviour of one dimensional and two dimensional systems are also quite distinct posing a challenge to the age-old ideas of the experimentalists and theoreticians.***

➢ ***The comparison of my derived spin stiffness constant with other theoretical and experimental results establishes the role of spin stiffness constant as effective exchange constants in both 1-D and 2-D systems.***

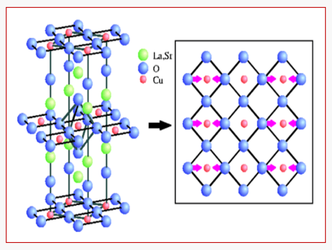
➢ ***A possible of point of quantum phase transition is seen near 61% doping concentration considering only the nearest neighbour hopping.***

➢ ***The possible point of phase transition is shifted to 15% doping concentration if the hopping involving two more near neighbours are considered. This is the region where the T_c is maximum for these high temperature superconductors.***

➢ ***Our formalism based on the quantum mechanical approach provides a straightforward way for calculating effective exchange constant for itinerant magnetic systems.***

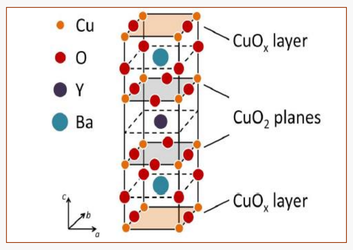
Motivation

The t-J model has been well established as one of the most important models for studying the antiferromagnetic doped insulators, which show high temperature superconductivity at optimal doping concentration. The study of the doped cuprates using t-J model also reveals the magnetic correlation present in the systems. This motivated us to investigate the connection of spin stiffness constant with effective exchange constant and charge stiffness constant with effective Coulomb interaction of one and two-dimensional antiferromagnets involving the rigorous analytic calculations on t-J model. The agreement with the previous experimental and theoretical results on the antiferromagnetic planes of La_2CuO_4 and oxygen deficient chains of $YBa_2Cu_3O_{6+x}$ added to the success of our result. The calculation of charge stiffness constant is going on and will be presented somewhere else in near future.



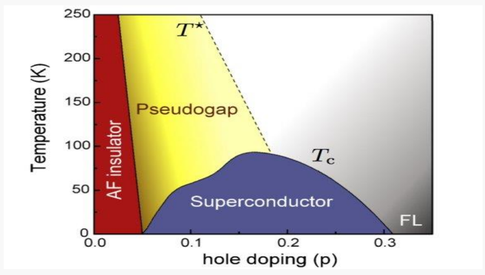
Structure of $La_{2-x}Sr_xCuO_4$

Fig.(1)



Structure of $YBa_2Cu_3O_{6+x}$

Fig.(2)



Phase diagram of hole-doped cuprates

Fig.(3)

Hubbard Model, t-J Model and t-t'-t''-J Model

The t-J model is a progeny model of the strongly correlated Hubbard model. The Hubbard model for the strongly correlated electrons consists of a hopping term and a on site Coulomb repulsion term.

The Hubbard Hamiltonian:-

$$H = H_{hop} + H_{int} \qquad (1)$$

This Hamiltonian takes the form:

$$H = -t\sum_{i,j,\sigma} C^{+}_{i\sigma} C_{j\sigma} + U\sum_{i} n_{i\uparrow} n_{i\downarrow} \qquad (2)$$

where t is the hopping probability amplitude from one site to another. $C_{i\sigma}(C^{+}_{i\sigma})$ is the Fermi annihilation (creation) operator for an electron at the site i with spin σ, and $n_{i\sigma} = C^{+}_{i\sigma}C_{i\sigma}$ is the number of electrons at a site with a given spin. The kinetic term is written in nearest-neighbor approximation for the transition matrix element, so that in this case the initial-band width W=2zt, where z is the number of nearest neighbour.

For U>>W, the second order perturbation in W/U gives the t-J model Hamiltonian for less than half-filled band band as -

$$H = -t\sum_{<i,j>,\sigma} C^{+}_{i\sigma} C_{j\sigma} + J\sum_{<i,j>} S_i \cdot S_j \qquad (3)$$

For, exactly half-filled band, the hopping part is zero and we get back the well-known Heisenberg model.

Now, the t-t'-t''-J model is given by:

$$H = -t\sum_{<i,j>,\sigma} C^{+}_{i\sigma} C_{j\sigma} - t'\sum_{<<i,j>>,\sigma} C^{+}_{i\sigma} C_{j\sigma} - t''\sum_{<<<i,j>>>,\sigma} C^{+}_{i\sigma} C_{j\sigma} + J\sum_{<i,j>} S_i \cdot S_j \qquad (4)$$

where 't' and 't'' are the next-nearest and next-next-nearest neighbour hopping amplitudes respectively.

Mathematical Formulation

The generalized spin stiffness constant is defined as [1]:

$$\tilde{D}_s = \lim_{\phi\to 0}\left(\frac{1}{2}\right)\frac{\delta^2 E}{\delta\phi^2} \qquad (5)$$

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

$$Ø_\downarrow = -Ø_\uparrow = Ø \qquad (6)$$

$\tilde{D}_s$ contains the contribution from both the hopping part ($\tilde{D}^t_s$) and the exchange energy part ($\tilde{D}^J_s$).

Hence, $$\tilde{D}_s = \tilde{D}^t_s + \tilde{D}^s_J \qquad (7)$$

The Gutzwiller state with variational parameter (α) set equal to 1 for completely projecting out the doubly occupied sites in the low doping regions:

Then, $$|\Psi_G\rangle = \prod_l (1 - n_{l\uparrow} n_{l\downarrow})|FS\rangle \qquad (8)$$

$$|\Psi_G\rangle_{NDOC} = \prod_l (1 - n_{l\uparrow} n_{l\downarrow}) \prod_{k,\sigma}\sum_{i,j} C^{+}_{i\sigma} C^{+}_{j-\sigma} e^{i(r_i - r_j).k}|vac\rangle \qquad (9)$$

Calculating the expectation values of energies in the normalized Gutzwiller state, the values of spin stiffness constants for two and one dimensional systems (taking only the nearest neighbour hopping) are summarized as [2]:

2-D

$$\tilde{D}^t_s = (-t)[\prod_{k,\sigma}^{k_F} 4\cos(k_x a)(1-\delta)^2 - N_l \prod_{k,\sigma}^{k_F} 4\cos(k_x a)/N^2] \qquad (10)$$

$$\tilde{D}^J_s = -4J\prod_{k}^{k_F} 2(1-\delta)^2 \qquad (11)$$

1-D

$$\tilde{D}^t_s = (-t)[\prod_{k,\sigma}^{k_F} 4\cos(ka)(1-\delta)^2 - N_l \prod_{k,\sigma}^{k_F} 4\cos(ka)/N^2] \qquad (12)$$

$$\tilde{D}^J_s = -4J\prod_{k}^{k_F} 2(1-\delta)^2 \qquad (13)$$

2-Dimension	1-Dimension
$\tilde{D}^t_s = 0$; for (i) n≥0.39 ie.,δ≤0.61 (ii) n→0 ie.,δ→1	$\tilde{D}^t_s = 0$; for (i) n=1 ie., δ=0 (ii) n→0 ie.,δ→1
$\tilde{D}^J_s = 0$; for (i) n→0 ie.,δ→1	$\tilde{D}^J_s = 0$; for (i) n→0 ie.,δ→1

Our recent calculations considering two next- nearest neighbour hoppings (t' and t'') along with 't' show that the generalized spin stiffness constant in 2-D due to hopping is:

$$\tilde{D}^t_s = (-t)[\prod_{k,\sigma}^{k_F} 4\{\cos(k_x a) + (t'/t)\cos(2k_x a) + (t''/t)\cos(3k_x a)\}(1-\delta)^2 - N_l \prod_{k,\sigma}^{k_F} 4\{\cos(k_x a) + (t'/t)\cos(2k_x a) + (t''/t)\cos(3k_x a)\}/N^2] \qquad (14)$$

The consideration of the next two nearest neighbour hoppings gives the non-zero expectation values of kinetic energy and $\tilde{D}^t_s$ just above ~15% doping concentration for proper choice of t' and t''. This is the possible point of possible phase transition where the doped insulators show the highest T_c (as shown in Fig. (3)).

The total generalized spin stiffness constant due to a pair of mobile holes is:

$$D_s = (\tilde{D}^J_s + \tilde{D}^t_s)/^{N_l} C_2 \qquad (15)$$

Previous experimental and theoretical results in 2-D

Neutron scattering experiment on $La_{2-x}Sr_xCuO_4$ above the corresponding Neel temperature gives the 2-D correlation length as function of doping concentration [2]:

Magnetic correlation length vs. strontium concentration, δ [Ref.(2),(3)].

Fig.(4)

$$\xi_{2D} = 3.8/\sqrt{\delta} \qquad (16)$$

Chakravarty, Halperin and Nelson (CHN) calculated the correlation length in 2D for pure Quantum Antiferromagnets using QNLσM at T→0K as [4]:

$$\xi_{2D} = C_{\xi}\exp[2\Pi\rho_s/k_B T] \qquad (17)$$

where $2\pi\rho_s$ is the spin wave stiffness constant

The 2-D correlation length for doped antiferromagnets from Quantum Monte Carlo study [5]:

Hence, $$\xi_{2D} = (0.276a/\sqrt{1-\delta})\exp[1.25J/T] \qquad (18)$$

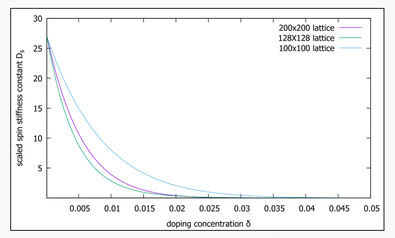
$$J_{eff} \sim \ln(0.075(\delta/1-\delta)) \qquad (19)$$

Himeda and Ogata calculated the effective antiferromagnetic exchange constant by introducing the effects of no double occupancy in the Gutzwiller factors [6]:

$$\tilde{t}_{eff} = g_t t \qquad \tilde{J}_{eff} = g_J J \qquad (20)$$

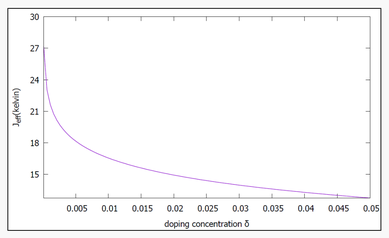
$$g_J = \frac{4(1-\delta)^2}{(1-\delta^2+4m^2)} \qquad (21)$$

Our results in 2-D based on t-J Model



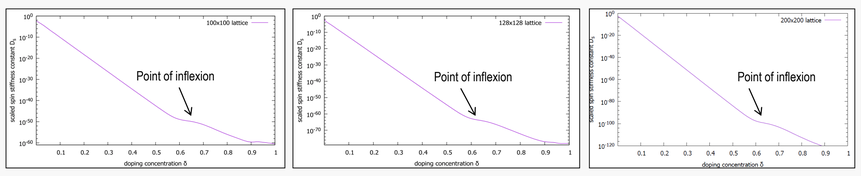
Scaled spin stiffness constant 'D_S' vs.doping concentration 'δ' plot upto 5% doping concentration with t ~ 8J ; for (a) 100x100, (b) 128x128, (c) 200x200 lattices [Ref.(2)]

Fig.(5a)



J_{eff} vs. doping concentration plot using equation (19) [Ref.(2)]

Fig(5b)

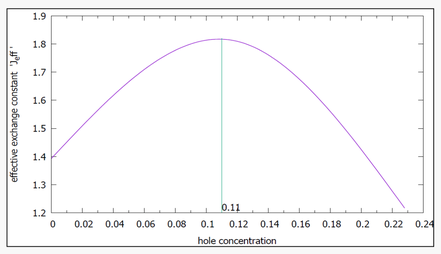


Scaled spin stiffness constant 'D_s' vs. doping concentration 'δ' plot upto 100% doping concentration in logscale; for (a) 100x100 ,(b) 128x128 , (c) 200x200 lattices [Ref.(2)]

Fig.(6)

Previous experimental results in 1-D

The susceptibility of $YBa_2Cu_3O_{6+x}$ was measured by Tranquada et al. by neutron scattering studies for various values of x[7]. The doping of oxygen introduces the holes only in the linear chains of $YBa_2Cu_3O_{6+x}$ upto $x \approx 0.4$ [8]. The effective spin stiffness constant (J_{eff}) is given by the inverse of dynamic susceptibility. J_{eff} of $YBa_2Cu_3O_{6+x}$ can be plotted against the doping concentration as:

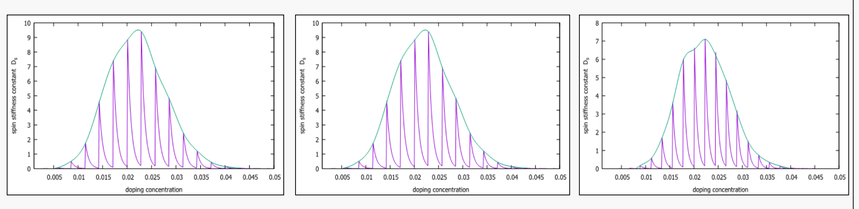


'J_{eff}' versus oxygen concentration 'x' at low temperature (~60K)

Fig(7)

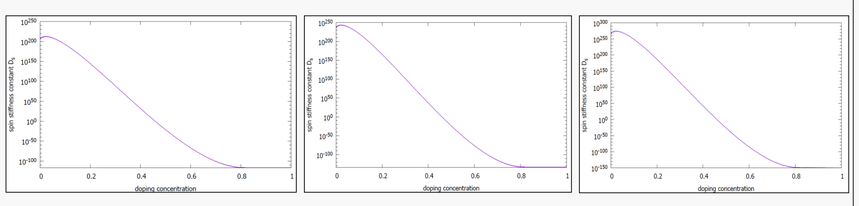
The peak seen here in the low doping concentration goes in well agreement with the presence of a peak in the envelope of our plot of spin stiffness constant

Our results in 1-D based on t-J model



Scaled spin stiffness constant 'D_s' versus doping concentration 'δ' plot upto 5% doping concentration with t~10J; for (a) 1400, (b) 1600, (c) 1800 lattices

Fig.(8)



Scaled spin stiffness constant versus doping concentration plot upto 100% doping concentration in logscale; for (a) 1400, (b) 1600, (c) 1800 lattices

Fig.(9)

Conclusion

The good agreement of our analytical results with the previous experimental and theoretical outcomes in both one and two dimensional systems once again establishes the paramount importance of t-J model in describing the doped antiferroamgnets[3,9-10]. The point of possible phase separation obtained nearly at 15% doping concentration considering next two nearest neighbours has importance in explaining the microscopic origin of high temperature superconductivity in the doped antiferromagnets in this doping region. The boundary of phase separation shown by Emery et al. for 2-D antiferromagnets is also relevant to our results[11]. The calculation of stiffness constant considering next two nearest neighbours is under process for 1-D antiferromagnets.

Moreover, our formalism paves a transparent way for studying the strongly correlated itinerant magnetic systems in the light of t-J model. The investigation of charge stiffness along with the spin stiffness can shed light on the pairing mechanism in these high temperature superconductors in the near future.

References

[1] *R.Chaudhury , J. Phys.: Condens. Matter **19**, 496203 (2007)*
[2] *S. Bhattacharjee, R. Chaudhury, Physica B **500,** 133-141 (2016)*
[3] *T.R. Thurston et al., Phy. Rev. B **40,** 4585 (1989)*
[4] S. Chakravarty et al., Phy. Rev B **39,** 2344 (1989)
[5] *E. Manousakis, Phy. Rev B **45,** 7570(R) (1992)*
[6] *A. Himeda, M. Ogata, Phys. Rev. B **60,** R9935(R) (1999)*
M. Ogata, A. Himeda, Preprint cond-mat/0003465 v1 (unpublished) (2000)
*A. Himeda, M. Ogata, Phys. Rev. Lett. **85**, 4345 (2000)*
[7] *J.M. Tranquada, A. H. Moudden, A.I. Goldman, P. Zolliker, D.E.Cox, G. Shirane, S.K. Sinha, D. Vaknin, D.C. Johnston, M.S. Alvarez, A.J. Jacobson, J.T. Lewandowski, J.M. Newsam, Phys. Rev. B **38**, 2477 (1988)*
[8] *N.M. Plakida, "High-Temperature Cuprate Superconductors" , chapter-III, "Springer Series in Solid State Physics", Springer Heidelberg London New York (2010)*
[9] *A.A. Vladimirov, D. Ilhe, N.M. Plakida, Phy. Rev. B **80,** 104425 (2009)*
[10] *A.A. Vladimirov, D. Ilhe, N.M. Plakida, Phy. Rev. B **83,** 024411 (2011)*
[11] *V.J. Emery, S.A. Kivelson, H.Q. Lin, Phys. Rev. Lett. **64**, 3562 (1990)*

Acknowledgement :- *I would like to acknowledge '**Inspire**' and '**S.N. Bose Centre**' for providing me with financial support and other facilities and my supervisor **Dr. Ranjan Chaudhury** for his guidance and suggestions for carrying out my research work.*