Magnetic correlation length for undoped and lightly doped La_2CuO_{4-y}

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We have used a self-consistent Green's function theory based on the quasi-two-dimensional Heisenberg model to explain the magnetic correlation length for both undoped and lightly doped samples of La_2CuO_{4-y}. Our analytical expression gives an exponential decay of correlation length with temperature and it includes the effect of doping through its dependence over the interlayer coupling. We have compared our numerical calculations with experimental results for magnetic correlation length in both undoped and lightly doped samples of La_2CuO_{4-y}. Our results are in excellent agreement with experimental results up to 900 K for the undoped compound.

I. INTRODUCTION

Spin correlations in both pure and doped cuprates show some very interesting magnetic properties, which have been the focus of attention lately.[1] Most of the magnetic properties in the insulating antiferromagnetic regime can be easily reconciled on the basis of a two-dimensional square-lattice Heisenberg antiferromagnetic model (2D-SLHAFM).[2] The real cuprates, however, are quasi-two-dimensional with a weak interlayer coupling which is responsible for the long-range order below the antiferromagnetic Néel temperature. The interlayer coupling for undoped La_2CuO_4 has been estimated to be of the order of 10^{-5}.[3] The effect of this weak but finite interlayer coupling towards the magnetic properties of these cuprates has been identified as extremely important and it affords us with a better understanding of the real systems.

Recently, the antiferromagnetic spin fluctuations have been studied with a variety of local as well as extended probes to find the spin correlation length in the cuprates.[4–6] Most informative among these experiments have been the neutron-scattering experiments since they cover the entire Brillouin zone and a wider range of energies. The neutron-scattering results of Keimer *et al.*[7] for the spin-spin correlation length in $La_{2-x}Sr_xCuO_4$ within the doping range $0 \leq x \leq 0.04$ have been one of the most comprehensive studies to date. They have shown that the magnetic correlation length is severely suppressed as a function of doping. Their results within the doping range $0.015 \leq x \leq 0.05$, which is referred to as the spin-glass state, shows various features which are similar to the AF state at x=0. Various other experiments prior to this one have also shown that the magnetic correlation length in undoped high-temperature superconductors decreases as the temperature is increased.[1,7–9] Birgeneau *et al.*[1] have shown that a tiny amount of hole concentration is enough to limit the correlation length. The correlation length was found to increase with decreasing temperature even in the presence of doped holes. Once it becomes comparable to the separation between two holes, it strongly suppresses the low-frequency part of the spin fluctuations as compared with the pure phase. All of these experiments were carried out for $T \leq 600$ K.

More recently however, the study of correlation length has been extended up to a temperature of 900 K by ^{63}Cu NMR and NQR experiments of Imai *et al.* on undoped and doped cuprates.[10] They have obtained the correlation length from the Gaussian component of the spin-spin relaxation rate for the undoped compound. Above 600 K, they show that the correlation length has an inverse linear dependence over temperature. Their results indicate that the growth of the antiferromagnetic correlation tends to saturate in the metallic region with decrease in temperature as soon as it becomes comparable to the average distance between two holes.

There have been numerous efforts to explain the magnetic correlation length for undoped compounds.[2,11–15] Chakravarty, Halperin, and Nelson[2] calculated the temperature dependence of the magnetic correlation length of a 2D spin-1/2 Heisenberg antiferromagnet by the renormalized group analysis of the Quantum nonlinear σ model. According to this theory the magnetic properties of the 2D Heisenberg antiferromagnet can be divided into two regimes in the paramagnetic state when the ground state is described as a Néel state. The temperature dependence of various properties in these two regimes are different from one another. In order to explain the experimental results of the correlation length, the expression for the renormalized classical regime ($2\rho_s \leq T \leq J$) was used and good agreement was obtained for pure La_2CuO_4. This theory was later modified by doing an exact analytic calculation including the first-order corrections in temperature by Hasenfratz and Niedermayer.[14] Recently, however, expressions for the spin-spin relaxation rate in the quantum critical regime of a 2D Heisenberg antiferromagnet have been used to fit the neutron-scattering results of the correlation length.[16] The Green's function method has also been used lately to study the correlation length in a 2D model[15] and a quasi-2D model by Majlis *et al.*[13] Majlis *et al.* have used a two-dimensional mean-field expression for the Néel temperature to evaluate the magnetic correlation length.

Various simulation studies have also been used to fit the experimental data for the correlation length. Manousakis[11] has obtained the magnetic correlation length by a direct simulation of the quantum nonlinear σ model. Manousakis has also pointed out that samples

with higher Néel temperature give different values of the correlation length. The correlation length via a large-scale Monte Carlo simulation on lattices up to 128×128 was done by Ding and Makivic.[12] They have, in their simulations, reached temperatures as low as $J/4$. Through their fits to the experimental data an estimate of $J = 1450 \pm 30$ K was obtained.

In this paper we have calculated the magnetic correlation length by using the Green's-function approach and a quasi-two-dimensional Heisenberg model.[13,15,17] We find an analytical expression for the correlation length in terms of the Néel temperature which depends crucially on the ratio of inter- to intraplanar exchange couplings. Our expression for the Néel temperature[18] is different than the mean-field expression and is consistent with the results of Mermin and Wagner.[19] We have used this expression to numerically evaluate the correlation length for the pure as well as lightly doped La compounds. Our results are in good agreement with the experimental results.

II. THEORY

We start with a quasi-two-dimensional Heisenberg antiferromagnet, with a weak three-dimensional interlayer coupling.[17,18] Below the Néel temperature, the interlayer coupling is responsible for the appearance of the long-range antiferromagnetic order in cuprates. The asymptotic form of the instantaneous spin-spin correlation function is used to obtain the correlation length. Following the method of Majlis *et al.*[13] and Yablonskiy[15] one obtains the following expression for the magnetic correlation length from the spin-spin correlation function:

$$\xi_c(r,T) \cong \frac{1}{C}\exp\left[\frac{D\,T_N(r)}{T}\right], \tag{1}$$

where $1/C = \delta_{ab}/4\sqrt{2}$ and $D = \zeta\,\pi/2$. Here, δ_{ab} is the lattice constant within the CuO_2 plane and ζ is a constant. $T_N(r)$ is the coupling-dependent Néel temperature. It is obtained from the expression of magnetization which has been evaluated by us using a Green's function theory and a quasi-two-dimensional Heisenberg model in Ref. 17. The self-consistent expression for the magnetization in terms of the spectral function $\rho(\omega)$ is given by[17]

$$M(T) = \frac{\mu g/2}{\int_0^1 d\omega\,[\rho(\omega)/\omega][1+2n_B(\omega E_0)]}. \tag{2}$$

n_B is the Bose distribution function and $E_0 = M(T)\,J_\parallel Z/\mu g$. The spectral function is defined as

$$\rho(\omega) = \omega\,D(\sqrt{1-\omega^2})/\sqrt{1-\omega^2}\,, \tag{3}$$

where $D(\omega)$ is given by

$$D(\omega) = \frac{2}{\pi N}\sum_q \mathrm{Im}\,\frac{1}{\omega-\gamma_q-i\delta}. \tag{4}$$

Here, $\gamma_q = (\cos q_x a + \cos q_y a + r\cos q_z c)/2 + r$ and r is the ratio of the inter- to intraplanar coupling strengths. By changing the summation over q by integration, the D function becomes

$$D(\omega) = \frac{4(2+r)}{\pi^3}\int_0^{\pi/2} F(\theta)d\theta$$

where

$$F(\theta) = K\left\{\sqrt{1-(\omega+r\omega/2-r/2+r\sin^2\theta)^2}\right\}. \tag{5}$$

Here K is the complete elliptic function of the first kind. Function D is the diagonal element of the generalized Watson function. We have calculated $T_N(r)$ appearing in Eq. (1) from Eq. (2), since for temperatures above the Néel temperature, the sublattice magnetization vanishes. We have calculated $M(T)$ vs T self-consistently by using Eqs. (2)–(5) and have found the value of $T_N(r)$ from this calculation.

Schwinger-boson mean-field theory (SBMFT) and spin-wave theory (SWT) are also used to calculate the Néel temperature in cuprates. Recently, Keimer *et al.*[20] have shown that for undoped cuprates SWT gives good results at low temperatures when the staggered magnetization is large whereas SBMFT is appropriate at higher temperatures when the staggered moment is sufficiently reduced. Both these theories, however, overestimate the Néel temperature in pure La_2CuO_4. On the other hand, we have shown that the self-consistent Green's function method is able to explain the temperature dependence of the magnetization over the entire temperature range.[18,21] Our self-consistent calculation gives Néel temperatures which are in excellent agreement with those obtained from experiments.[18,21] In this method, the dependence of T_N over the interlayer coupling is given by $T_N \propto [1 + C\ln(1/r)]^{-1}$, where C is a constant. A similar expression has also been obtained by Majlis *et al.*[13] In retrospect, both SBMFT and SWT give $T_N \propto [\ln(1/r)]^{-1}$.[20,22]

III. RESULTS AND DISCUSSION

Our expression of the magnetic correlation length contains a Néel temperature which is dependent on the ratio of inter- to intralayer exchange couplings. It has been shown that varying the coupling ratio changes the Néel temperature in these compounds. We have also established that a linear dependence of the coupling ratio over the doping concentration can suitably explain the effect of moderate dopings on magnetic properties in cuprates.[18] There have been a few recent attempts to study the doping dependence of the correlation length. Keimer *et al.*[7] have used a generic mean-field expression for undoped samples and a simple relation to fit their neutron-scattering results for four doped samples of $La_{2-x}Sr_xCuO_{4-y}$. Majlis *et al.*[13] have taken the mean-field theory to evaluate the Néel temperature. In apparent contrast to these results our expression for the magnetic correlation length is more suited for both lightly doped and undoped superconductors since it depends upon the doping concentration through the interlayer ex-

change coupling.

We have calculated the magnetic correlation length for the undoped and oxygen-doped sample of La_2CuO_{4-y} compounds. In Fig. 1, we show the variation of the inverse correlation length with temperature for undoped materials within the temperature range $T_N \leq T \leq 900$ K. Such high temperatures have been experimentally inaccessible until very recently. Imai *et al.*[10] have used ^{63}NMR and NQR techniques to measure the spin-lattice relaxation and spin-echo decay rate in undoped cuprates. They have derived the magnetic correlation length from the measured values of the Gaussian component of the spin-echo decay rate. They have shown that within the temperature range 600–900 K the inverse correlation length has an inverse linear temperature dependence. We have calculated the magnetic correlation length from Eq. (1) with $J_{\|} = 0.130$ eV and $r = 1.0 \times 10^{-5}$, which are close to the values reported for undoped La_2CuO_4.[3] The Néel temperature calculated with these values for the undoped compound is 318 K, which is in excellent agreement with the experimental results of Keimer *et al.*[7] The Néel temperature is evaluated through $M(T)$ self-consistently.[21]

Further, we have put $C \sim 4\sqrt{2}/\delta_{ab}$ and have varied D to obtain good agreement with experimental results. Here, $\delta_{ab} \sim 3.8$ Å. Having obtained the theoretical values of the magnetic correlation length for an undoped La compound, we have compared it with the experimental results of Imai *et al.*[10] We have shown that although the slope of the theoretical curve is in excellent agreement with the data of Imai *et al.* there is a slight difference between the magnitudes. Yet, the nature of the theoretical curve and the experimental results are consistent with each other. The experimental data points at least below 600 K, taken from Keimer *et al.*,[7] that we have plotted here, do not contain the relatively large error bars. Having that in mind, our theoretical results are in excellent agreement with the experiments both qualitatively and quantitatively.

Figure 2 shows the variation of the inverse magnetic correlation length for oxygen-doped and undoped samples of La_2CuO_{4-y}. The open and solid circles represent

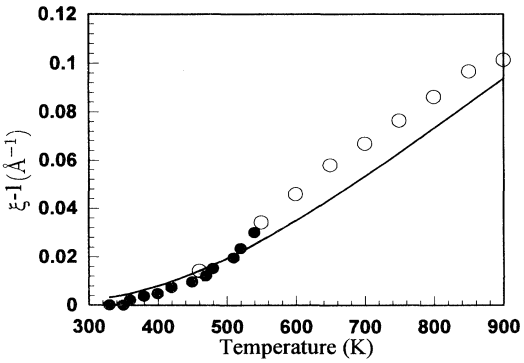

FIG. 1. Variation of ξ^{-1} with T for undoped La_2CuO_4. The experimental results are taken from Keimer *et al.* (○) and Imai *et al.* (●).

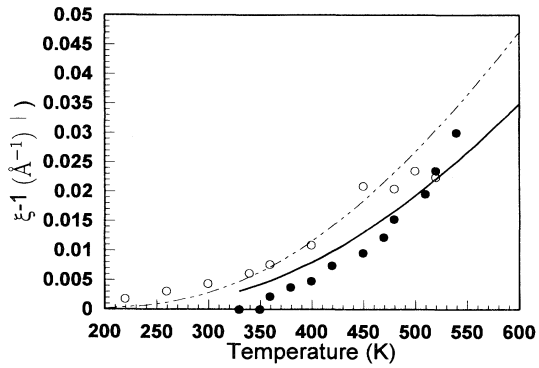

FIG. 2. Variation of ξ^{-1} with T for undoped and doped samples of La_2CuO_{4-y}. Experimental results from Keimer *et al.* for the oxygen-doped sample ($T_N = 190$ K) are denoted by (○) while experimental results for the undoped ($T_N = 325$ K) sample are denoted by (●). Lines represent the theoretical results, as discussed in text.

the experimental results for oxygen-doped and undoped samples of La_2CuO_{4-y} obtained from neutron-scattering experiments of Keimer *et al.*[7] Again, we have omitted the error bars in the experimental data. For the doped sample La_2CuO_{4-y}, with a hole concentration of 0.01, the experimental Néel temperature is 190 K. In our theory, the doping dependence of the Néel temperature comes through the interlayer coupling.[18,23] Using the experimental Néel temperature (190 K for the doped sample), we have calculated the interlayer coupling by evaluating Eq. (2) self-consistently. It is found that $r \sim 1 \times 10^{-7}$. Hence a doped sample with a hole concentration of 0.01 corresponds to an interlayer coupling of 10^{-7} in our theory. For this sample, we have chosen C=1.27 and D=8.909 to calculate the magnetic correlation length while for the undoped sample C=1.48 and D=5.62, the same as in Fig. 1. The numerical results are presented in Fig. 2 where the curves are obtained from our expression for correlation length [cf. Eq. (1)].

It is evident from the figure that with these values for C and D, the experimental results can be easily explained. The value of C, for the undoped compound is obtained from the theory, however a decrease in the value of C for the doped compound can be justified by the following arguments. (i) When these cuprates are doped with oxygen, they take up sites between two copper atoms in the CuO_2 planes. Therefore, this doping would slightly enhance the separation between the copper atoms. (ii) It may be possible that C does depend explicitly on the doping concentration and is a function of x or y or both. Our theory is not able to produce this doping dependence of C in doped cuprates. According to these arguments, the variation of C with doping should be very small. Barring this relatively small effect of doping on the value of C, our theoretical results can explain the experimental data of Keimer *et al.*

In order to put our results into proper perspective, let us compare our results with the simulation studies. So far, one of the most accurate simulation studies performed on the spin-1/2 quantum Heisenberg antiferro-

magnet, by Ding and Makivic,[12] has found that their numerical data can be best fitted by an expression of the kind $\xi = 0.27a \exp[\frac{1.25J}{T}]$. If we compare our theoretical results with these simulation results, we find that there is a correspondence between our theory and the expression given above. According to our calculations, $0.27a$ in the expression above is replaced by a constant $1/C$ while $1.25J$ is replaced by DT_N. Our numerical results have shown that $1/C = 0.68$ while simulation results have a value of 1.1 ($\sim 0.27a$). Our estimates give a value of DT_N=1800 K while the simulation results give 1875 K ($1.25J$) for the same value of planar exchange couplings. Again, the theoretical expression is in very good agreement with the Monte Carlo simulation results.

In conclusion, by considering a quasi-two-dimensional Heisenberg model and using the many-body Green's-function approach, we have found an expression for the magnetic correlation length which is dependent on the coupling ratio. This expression has been used to numerically evaluate the magnetic correlation length for both undoped and oxygen-doped samples of La_2CuO_{4-y}. We have compared our theoretical results with the neutron-scattering results for both undoped and doped samples. At elevated temperatures ($600 < T < 900$ K), the theoretical results are able to explain the recent experimental results.

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