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Microscopic calculation of the spin-stiffness constant for the spin-$\frac{1}{2}$ square-lattice Heisenberg antiferromagnet

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We discuss a systematic, microscopic calculation of the spin-stiffness constant ρ_s for the spin-$\frac{1}{2}$ square-lattice Heisenberg antiferromagnet. An infinitesimal twist is imposed upon the system by gradually rotating the direction of antiferromagnetic ordering. The difference in the ground-state energy of this system with respect to the uniformly ordered ground state can be related to the spin-stiffness constant ρ_s. Series expansions and extrapolation for the energy of the twisted system lead to the estimate $Z_{\rho_s}(=4\rho_s/J)=0.72\pm0.04$. The ratio of the series for ρ_s and perpendicular susceptibility $\chi_\perp$ leads to an estimate for the spin-wave velocity c_s of $Z_{c_s}(=c_s/\sqrt{2}J)=1.18\pm0.02$. The experiments on La_2CuO_4 are quantitatively consistent with a nearest-neighbor Heisenberg model when one takes into account these quantum renormalizations.

Recently there has been much interest in understanding the low-temperature static[1] and dynamic[2,3] properties of Heisenberg antiferromagnets. Underlying any macroscopic description of these systems are the questions of long-range order and the microscopic determination of the parameters such as the sublattice magnetization M^+, the spin-stiffness constant ρ_s, the transverse susceptibility $\chi_\perp$, and the spin-wave velocity c_s. In previous papers[4–7] we have shown that series expansions and extrapolations around various ordered and disordered exactly soluble Hamiltonians provide a systematic way of understanding the ground-state properties of these systems. In particular, expansions around the disordered ground states of dimerized Hamiltonians suggest a spontaneous development of Néel order for the uniformly coupled square-lattice nearest-neighbor (NN) spin-$\frac{1}{2}$ Heisenberg antiferromagnet.[5] In complete agreement with this conclusion, the expansion around the ordered ground state of the Ising Hamiltonian suggests that for the Heisenberg model M^+ is reduced but not eliminated by quantum fluctuations.[4,6] Thus, the Ising expansions are convergent up to the Heisenberg point, and, hence, provide a basis for a systematic determination of the above parameters. The power series thus obtained are, however, singular due to the existence of gapless spin-wave excitations at the Heisenberg point. Nevertheless, borrowing series extrapolation techniques from the study of classical critical phenomena they can be used to estimate these parameters accurately.

It is the purpose of this paper to explain how the spin-stiffness constant ρ_s, and hence the spin-wave velocity c_s, can be estimated by series expansions around the Ising limit. The extrapolated estimates have been reported previously.[6] ρ_s is defined in terms of the energy required to impose an infinitesimal twist on the system. Our calculation involves rotating the direction of antiferromagnetic ordering gradually in space and calculating the energy of the imposed twist. In order to obtain this energy, we rotate the axis of quantization, and thus the direction of ordering, gradually in space and express the Heisenberg Hamiltonian in terms of the rotated spin variables. We can now perform Ising expansions for the ground-state energy of this system in the variable $J_\perp/J_\parallel$, where $J_\parallel$ is the coupling parallel to the direction of ordering, and $J_\perp$ the coupling perpendicular to it. Our calculation, thus, illustrates a general principle that can be used to develop Ising-type expansions for systems which may have noncolinearly ordered ground states, such as the triangular-lattice Heisenberg model. Finally, the ratio of the series for ρ_s and $\chi_\perp$ is used to estimate the spin-wave velocity c_s.

The summation of these series, to estimate the parameters of the Heisenberg model, is guided by the spin-wave theory.[8] This theory not only gives us the exact values for the exponents of the singularities in ρ_s and c_s at the Heisenberg point ($J_\perp/J_\parallel=1$), but also some suitably defined universal amplitude ratios.[6] These turn out to be very useful in an accurate determination of these parameters.

Let us begin with the definition of the spin-stiffness constant or helicity modulus ρ_s. If we rotate the order parameter of a magnetically ordered thermodynamic system by an angle θ per unit length then the ground-state energy of the system, per lattice site, is increased to

$$E(\theta)=E(\theta=0)+\tfrac{1}{2}\rho_s\theta^2+O(\theta^4)\ . \tag{1}$$

For example, let us first consider the classical Heisenberg Hamiltonian with spin S on a square lattice,

$$H=J\sum_i \mathbf{S}_i\cdot[\mathbf{S}_{i+\hat{\mathbf{x}}}+\mathbf{S}_{i+\hat{\mathbf{y}}}]\ , \tag{2}$$

where $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ are unit distances to the nearest neighbors in the x and y directions. Applying a twist θ per lattice constant along the y direction (so $\mathbf{S}_i=-\mathbf{S}_{i+\hat{\mathbf{x}}}$ and $\mathbf{S}_i\cdot\mathbf{S}_{i+\hat{\mathbf{y}}}=-S^2\cos\theta$), the energy per lattice site becomes

$$E(\theta)=J(1+\cos\theta)(-S^2)\ , \tag{3}$$

so that the spin-stiffness constant is

$$\rho_s = JS^2 \ . \tag{4}$$

To estimate ρ_s for the $S=\frac{1}{2}$ quantum system we rotate the axis of quantization by a relative angle θ for the neighboring sites along the y direction. (The rotation being about the y axis in spin space.) In terms of the rotated spin variables, $\{\sigma_i\}$, the Hamiltonian becomes

$$\begin{aligned} H = J\sum_{\langle ij\rangle} \mathbf{S}_i\cdot\mathbf{S}_j &= \frac{J}{4}\sum_i [\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_{i+\hat{x}} + \sigma_i^y\sigma_{i+\hat{y}}^y + \sigma_i^x[\sigma_{i+\hat{y}}^x\cos\theta + \sigma_{i+\hat{y}}^z\sin\theta] + \sigma_i^z[-\sigma_{i+\hat{y}}^x\sin\theta + \sigma_{i+\hat{y}}^z\cos\theta]] \\ &= \frac{J}{4}\left[\sum_i \boldsymbol{\sigma}_i\cdot[\boldsymbol{\sigma}_{i+\hat{x}} + \boldsymbol{\sigma}_{i+\hat{y}}] + (\cos\theta-1)\sum_i(\sigma_i^x\sigma_{i+\hat{y}}^x + \sigma_i^z\sigma_{i+\hat{y}}^z) + \sin\theta\sum_i(\sigma_i^x\sigma_{i+\hat{y}}^z - \sigma_i^z\sigma_{i+\hat{y}}^x)\right] , \end{aligned} \tag{5}$$

where the $\{\boldsymbol{\sigma}_i\}$ are Pauli spins (normalized so $\sigma_i^2=3$). We would like to compute the energy of this system with the spins $\boldsymbol{\sigma}$ ordered antiferromagnetically along the z axis, the original spins $\mathbf{S}$ are twisted when the spins $\boldsymbol{\sigma}$ are uniform. Since the definition of ρ_s requires the computation of the ground-state energy only to order θ^2, we expand the cosine and sine in powers of θ to get

$$\begin{aligned} H = \frac{J}{4}\Bigg[&\sum_i \boldsymbol{\sigma}_i\cdot(\boldsymbol{\sigma}_{i+\hat{x}} + \boldsymbol{\sigma}_{i+\hat{y}}) - \tfrac{1}{2}\theta^2\sum_i(\sigma_i^x\sigma_{i+\hat{y}}^x + \sigma_i^z\sigma_{i+\hat{y}}^z) \\ &+ \theta\sum_i(\sigma_i^x\sigma_{i+\hat{y}}^z - \sigma_i^z\sigma_{i+\hat{y}}^x)\Bigg] + O(\theta^3) \ . \end{aligned} \tag{6}$$

The second term is already of order θ^2 so it can be replaced by its expectation value in the ground state of the $\theta=0$ Hamiltonian. The contribution of the third term to the ground-state energy in order θ^2 can be obtained by treating it in second-order perturbation theory. Thus we consider the Hamiltonian

$$H_\theta = \frac{J}{4}\left[\sum_{\langle ij\rangle}\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j + \theta\sum_i \sigma_i^z(\sigma_{i-\hat{y}}^x - \sigma_{i+\hat{y}}^x)\right] , \tag{7}$$

where the first term runs over all nearest-neighbor pairs, and we have rearranged the θ term from the previous expression.

Let the ground-state energy per site of the Hamiltonian H_θ be

$$E_\theta = E(\theta=O) + \widetilde{E}_\theta\theta^2 + O(\theta^3) \ . \tag{8}$$

Then ρ_s is given by the expression

$$\tfrac{1}{2}\rho_s = -\tfrac{1}{2}J\sum_i\langle s_i^x s_{i+\hat{y}}^x + s_i^z s_{i+\hat{y}}^z\rangle + \widetilde{E}_\theta \ . \tag{9}$$

Here the angular brackets represent the expectation value in the unperturbed ground state with the spins ordered along the z axis. Our aim now is to develop perturbation expansions for the terms on the right-hand side of this expression. In order to do this we add another parameter to H_θ, defining

$$\begin{aligned} H'_\theta = \sum_{\langle ij\rangle}&\left[\frac{J_\parallel}{4}\sigma_i^z\sigma_j^z + \frac{J_\perp}{4}\boldsymbol{\sigma}_i^\perp\cdot\boldsymbol{\sigma}_j^\perp\right] \\ &+ \frac{J_\parallel\theta}{4}\sum_i\sigma_i^z(\sigma_{i-\hat{y}}^x - \sigma_{i+\hat{y}}^x) \ , \end{aligned} \tag{10}$$

where $\boldsymbol{\sigma}^\perp$ constitutes the x and y components of $\boldsymbol{\sigma}$. The Heisenberg model is $J_\perp=J_\parallel$, while $J_\perp=0$ is an Ising model for which the ρ_s defined by (9) is simply calculated. We then develop a perturbation expansion for this ρ_s in powers of $x\equiv J_\perp/J_\parallel$.

The expansions are developed by the method of Singh, Gelfand, and Huse.[5] The only new feature is that the 90° rotational symmetry of the lattice is broken by the imposed twist in the Hamiltonian. This leads to additional diagrams compared to those needed in Ref. 6 for $\chi_\perp$ or M^+.

It is common to express ρ_s and c_s in terms of a multiplicative renormalization of the classical answer. Thus, we obtain the expansions (giving four significant digits)

$$\begin{aligned} Z_{\rho_s} = \left[\frac{4\rho_s}{J}\right] &= 1 - \tfrac{1}{18}x^2 - \tfrac{1}{18}x^3 - 0.016\,85x^4 \\ &\quad - 0.004\,394x^5 \\ &\quad - 0.013\,06x^6 - 0.007\,554x^7 \ . \end{aligned} \tag{11}$$

Furthermore, a similar renormalization for $\chi_\perp$ is given by[6]

$$\begin{aligned} Z_\chi = 8\chi_\perp J &= 2 - \tfrac{8}{3}x + \tfrac{17}{6}x^2 - \tfrac{82}{27}x^3 + 3.068x^4 \\ &\quad - 3.145x^5 + 3.167x^6 - 3.223x^7 \ . \end{aligned} \tag{12}$$

From these two, and the assumption of standard antiferromagnetic hydrodynamics in the Heisenberg model, a series that extrapolates to the spin-wave velocity at $x=1$ can be obtained through the relation $Z_c^2 = Z_{\rho_s}/Z_{\chi_\perp}$.

Before we analyze these series, we need to consider the structure of the singularity at the Heisenberg point $x=1$. We know from spin-wave theory[8] that the quantities Z_{ρ_s}, Z_χ, Z_{c_s}, etc., have singularities at $x=1$ caused by the closing of the gap for the Goldstone mode (spin waves). Furthermore, the form of the singularities has to be of the type $(1-x)^{m+1/2}$ with $m=0,1,2,\ldots$, etc. The amplitude for the leading (square-root) singularity should be universal if appropriate dimensional factors are scaled out. Thus, if we separate the singular parts at $x=1$ via

$$\rho_s = \rho_s^0 + \rho^{\text{sing}}, \quad \chi_\perp = \chi_\perp^0 + \chi_\perp^{\text{sing}} \ , \tag{13}$$

then

$$R = \lim_{x\to 1}(\rho_s^{\text{sing}}/\rho_s^0)/(\chi_\perp^{\text{sing}}/\chi_\perp^0) \ , \tag{14}$$

should be universal, independent of short-distance properties such as spin, etc.

A spin-wave estimate can be obtained for the expression in Eq. (14) through the Holstein-Primakoff transformation. The $S \to \infty$ limit for ρ_s and its leading (square-root) singularity come entirely from the first term in a $1/S$ expansion. It then follows from a straightforward calculation that $R=1$. That $\chi_\perp$ and ρ_s have the same relative singularities is not surprising since they play essentially identical roles as coefficients of the gradient-squared terms in the (2+1)-dimensional nonlinear σ-model description of this system.[1]

Since the series for c_s^2 is the ratio of the series for ρ_s and $\chi_\perp$ it follows that the amplitude for the square-root singularity in c_s^2 must vanish identically. Thus, the leading singularity that needs to be taken into account in extrapolating c_s^2 should be of the form $(1-x)^{3/2}$. This is a definite prediction from the hypothesis of universal (independent of S) amplitude ratios, which can, in principle, be checked through the series.

Since the quantities Z_χ and Z_{ρ_s} have competing singularities at $x=\pm 1$, we go to a new variable which moves the singularity at $x=-1$ to infinity. This new variable is

$$z=2x/(1+x) \ .$$

In this variable, the series become

$$Z_{\rho_s}=1+0z-0.0138z^2-0.020\,83z^2-0.021\,89z^4$$
$$-0.019\,60z^5-0.016\,20z^6-0.012\,93z^7 \ ,$$
$$(Z_c)^2=\tfrac{1}{2}+\tfrac{1}{3}z+0.2049z^2+0.1204z^2+0.069\,08z^4$$
$$+0.039\,75z^5+0.023\,73z^6+0.015\,25z^7+\cdots \ .$$

In order to sum these series at the Heisenberg point, we construct the sums S_N given by[6]

$$S_N=\sum_{n=0}^{N} a_n x^n \ .$$

Then, asymptotically (as $N \to \infty$)

$$S_N \approx S_\infty + \frac{C}{(N+\alpha)^\lambda} + O(N^{-(2+\lambda)}) \ ,$$

where S_∞ is the sum of the infinite series, λ the exponent, C the amplitude of the leading singularity, and α depends on the amplitude of the next to leading singularity. The ratio of C to S_∞ for two different quantities, such as ρ_s and $\chi_\perp$ is determined by the criterion of universal amplitude ratios. Hence, to estimate these quantities we plot the partial sum S_N versus $1/(N+\alpha)^\lambda$ for different α and choose a value of α such that $R=1$ to get the best estimate for ρ_s. The plot is shown in Fig. 1, while that for $\chi_\perp$ is in Ref. 6. We obtain

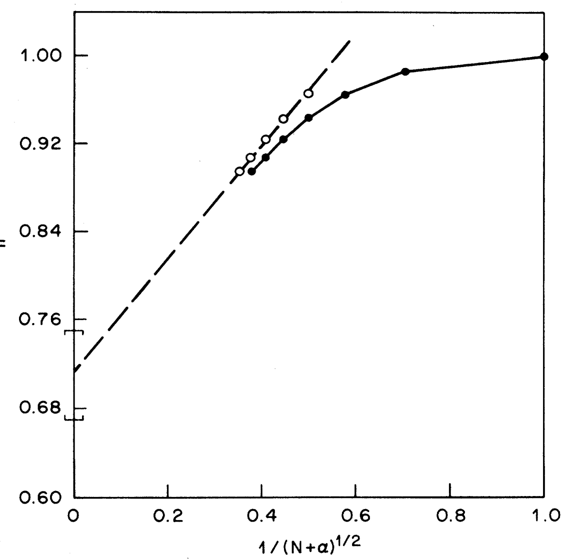

FIG. 1. Plots of partial sum S_N for Z_{ρ_s} vs $1/(N+\alpha)^{1/2}$ where N is the number of terms in the series. The solid circles correspond to $\alpha=0$, while the open circles correspond to $\alpha=1$. The latter is chosen to get the ratio R in Eq. (14) equal to unity. The dashed line is a least-squares fit to the points. The extrapolated estimate (S_∞) is shown by brackets.

$$Z_{\rho_s}=0.71\pm 0.04 \ .$$

Alternatively, ρ_s can also be estimated by employing the change of variables (Ref. 4) $1-\delta=\sqrt{1-z}$ to get a series in δ which is free of singularities at the Heisenberg point ($\delta=1$). We can then use ordinary Padé approximants to sum the series. The Padé estimates are shown in Table I. From these we estimate

$$Z_{\rho_s}=0.73\pm 0.04 \ ,$$

where the uncertainties reflect the spread in the Padé es-

TABLE I. Padé estimates for Z_{ρ_s} in the variable δ. An asterisk indicates a singularity on the real axis in the range $0<\delta<1$.

M/N	0	1	2	3	4	5	6	7
0	1.0	1.0	0.94	0.83	0.72	0.67	0.69	0.76
1	1.0		1.06*	5.12*	0.62	0.69	0.65*	
2		1.06*	0.94	0.87	0.79	0.76		
3	0.86	−1.01*	0.87	2.39*	0.70			
4	0.78	0.70	0.80	0.70				
5	0.74	0.74	0.77					
6	0.74	0.74*						
7	0.76							

timates. Thus the two different methods lead to estimates which are consistent with each other.

To compare with other evaluations of ρ_s, we note that the order $1/S$ expansion of the spin-wave theory[1,8] gives $Z_{\rho_s} \simeq 0.60$, while the Schwinger boson mean-field theory[2] gives $Z_{\rho_s} \simeq 0.71$. Thus our results are in excellent agreement with that of Schwinger boson mean-field theory.

To get the estimate for the renormalization of the spin-wave velocity we plot the partial sums versus both $1/N^{1/2}$ and $1/N^{3/2}$ (see Fig. 2). We see that the plot versus $1/N^{3/2}$ settles down to a nice straight line, thus validating the assumption of universal amplitude ratios, which suggests that the amplitude for the square-root singularity for Z_c must vanish. Thus, we estimate

$$Z_c^2 = 1.38 \pm 0.04 .$$

This estimate is quite close to that obtained in the $1/S$ expansion by Oguchi,[8] and in Schwinger boson mean-field theory.[3] In both cases the value is $Z_c^2 \simeq 1.35$.

We are now in a position to compare these estimates against experiments on La_2CuO_4. We first note that the exchange constant J for La_2CuO_4 has been accurately obtained by comparing the frequency moments of the observed two-magnon light scattering spectra to that estimated by Ising expansions.[7] This leads to $J = 1500 \pm 75$ K. Furthermore, the slope of the spin-wave (magnon) dispersion near the antiferromagnetic zone center has been measured directly by neutron scattering,[9] leading to an estimate for the spin-wave velocity, c_s. Using the renormalization Z_{c_s} computed above, this leads to an estimate of $J = 1550 \pm 60$ K. The quantity ρ_s can also be measured directly through experiments as it controls the exponential growth of the correlation length above the three-dimensional ordering temperature

$$\xi \approx A e^{(2\pi\rho_s)/(k_B T)} \equiv A e^{(\pi Z_{\rho_s} J)/(2k_B T)} .$$

Here, the prefactor A is a slowly varying function of temperature. Because the estimation of ρ_s requires fitting the data above the Néel temperature to this form, the uncertainties are large. For ξ deduced from the Brookhaven susceptibility data,[10] Chakravarty, Halperin, and Nelson find $J \approx 1200$ K assuming $Z_{\rho_s} \simeq 0.60$ (the spin-wave estimate). In an independent fit Gomez-Santos, Joannopoulos, and Negele[11] find the data to be consistent with $Z_{\rho_s} \approx 0.63$ and $J = 1600$ K. The latter implies that the data is also consistent with $Z_{\rho_s} = 0.7$ and $J = 1500$ K. It should be noted that the Néel temperature for the Brookhaven sample is 195 K instead of 265 K for the other two measurements, and hence it can have a somewhat smaller J value, due to sample preparation.

An interesting question that arises is: To what extent does the nearest-neighbor Heisenberg model quantitatively describe La_2CuO_4, and what role, if any, is played by frustrating further-neighbor interactions?

The comparison of various frequency moments of the inelastic light scattering spectra[7] against those computed theoretically for the NN Heisenberg model agreed to an accuracy of 10%. This suggests that short-wavelength fluctuations are quantitatively accounted for, to this accuracy, by this model. The measured long-wavelength spin-wave velocity[9] is also in excellent agreement with the renormalization expected for the NN Heisenberg model, assuming J is taken from the two-magnon light scattering experiments. Thus, the shape of the full spin-

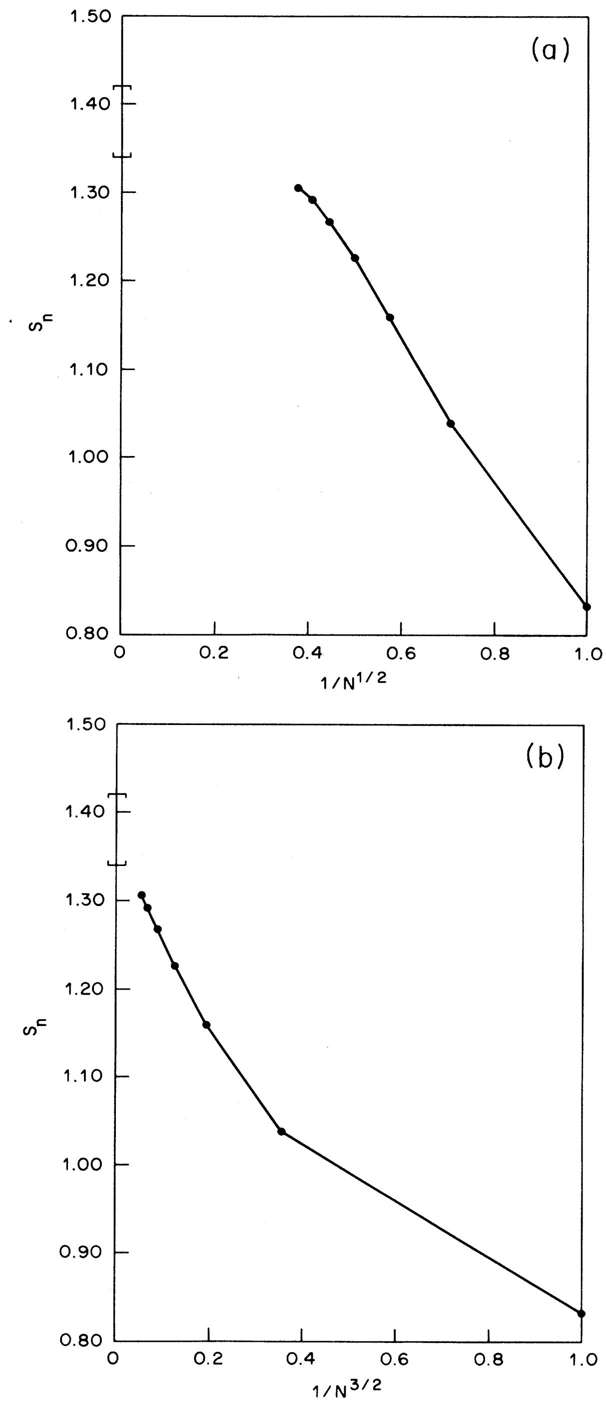

FIG. 2. Plots of partial sum S_N for Z_c^2 (a) vs $1/N^{1/2}$, (b) vs $1/N^{3/2}$. If the leading singularity for Z_c^2 goes as $(1-x)^{3/2}$ then the plot vs $1/N^{1/2}$ should approach the Y axis at 90°.

wave dispersion curve must agree reasonably well with that of a NN Heisenberg model. The estimates of Z_{ρ_s}, from the temperature dependence of ξ, are also consistent (within large uncertainties) with the estimates for the NN model. However, to the extent that one obtains a somewhat smaller Z_{ρ_s} than expected for the NN Heisenberg model, it gives us a measure of the amount of frustration in this system. Let us remember that with sufficient frustration (for example, due to second- or third-neighbor interactions) the system may be disordered at $T=0$. At this point[1] $Z_{\rho_s} \rightarrow 0$, $Z_\chi \rightarrow 0$, whereas Z_{c_s} remains finite, and presumably the entire spin-wave dispersion curve is not drastically altered. Thus the relative reduction in Z_{ρ_s} or Z_χ with respect to Z_{c_s} is a measure of the significance of further-neighbor interaction in the system. Thus a combined measurement of the $T=0$ spin-wave velocity and the temperature dependence of ξ on the same sample could, in principle, serve to constrain the amount of frustration in the system.

To summarize, we have presented here a systematic microscopic calculation of the spin-stiffness constant ρ_s, and the spin-wave velocity c_s, for the $T=0$, NN spin-$\frac{1}{2}$ square-lattice Heisenberg antiferromagnet. The estimate for Z_{ρ_s} (0.72±0.04) differs from the order $1/S$ spin-wave value (0.60) by about 15%, while that for Z_{c_s} (1.18±0.02) is very close to it (1.16). Both these estimates are remarkably close to the Schwinger boson mean-field theory ($Z_{\rho_s}=0.71$, $Z_{c_s}=1.16$). The estimated quantum renormalizations provide a quantitatively consistent picture for the experiments on La_2CuO_4.

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