Direct calculation of spin stiffness for spin-$\frac{1}{2}$ Heisenberg models

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The spin stiffness of frustrated spin-$\frac{1}{2}$ Heisenberg models in one and two dimensions is computed by exact diagonalizations on small clusters that implement spin-dependent twisted boundary conditions. Finite-size extrapolation to the thermodynamic limit yields a value of 0.14 ± 0.01 for the spin stiffness of the unfrustrated planar antiferromagnet. We also present a general discussion of the linear-response theory for spin twists, which ultimately leads to the moment sum rule.

One of the most basic questions in the study of magnetism is that of the existence or absence of long-range order in the corresponding magnetic moments. A partial answer to this question can be given by the determination of the so-called spin stiffness of the magnet, which measure the rigidity of the spins with respect to a small twist. In particular, systems possessing long-range spin order are stiff, while spin systems that are not stiff accordingly show no long-range order in the moments. In the case of spin-$\frac{1}{2}$ systems, the latter stiffness can be directly measured by the generation of a spin current with a spin-dependent magnetic field, as was shown by Shastry and Sutherland.[1] This method is analogous to that used to measure the charge stiffness of a system,[2] which discriminates between metals and insulators.

In this paper, we apply the former method to the case of the spin-$\frac{1}{2}$ Heisenberg model, $H_0 = \sum_{(i,j)} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$, on both chain and square-lattice geometries. First, we give a general discussion of spin twists for this model based on linear-response theory, which ultimately leads to the moment sum rule.[3] We then make practical use of the above method to measure the spin stiffness of near-neighbor Heisenberg chains and square lattices by exact diagonalization of the $S_z = 0$ subspace with the Lanczos technique.[4] Employing finite-size extrapolations, we find values of the spin stiffness for the nearest-neighbor Heisenberg ferromagnet and antiferromagnet on the square lattice that agree with spin-wave theory results to within 10%.[5] In the particular case of the square lattice, where reported results for this quantity vary widely,[6] we obtain an upper bound for the spin stiffness of $\rho_s/J \cong 0.174$, as well as an extrapolated value of $\rho_s/J = 0.14\pm0.01$ in the thermodynamic limit. Also, for the case of spin-$\frac{1}{2}$ frustrated antiferromagnets with next (next) nearest-neighbor interactions, we generally find that the stiffness coefficient vanishes near the point where the analogous classical model losses long-range order in the magnetic moments.[7] We now turn to the derivation of the moment sum rule.

Linear-response. Following Ref. 1, the rigidity of a Heisenberg model with respect to a twist about the spin z axis is reflected in the ground-state energy of the modified Hamiltonian,

$$H = \sum_{(i,j)} J_{ij} [\tfrac{1}{2}(S_i^+ S_j^- e^{i\theta_{ij}} + S_i^- S_j^+ e^{-i\theta_{ij}}) + S_i^z S_j^z] , \quad (1)$$

where θ_{ij} represents the twist angle on the bond (i,j). Hence, in the limit of small twists, the above Hamiltonian is expressible as $H = H_0 + H_1$, where H_0 represents the unperturbed Heisenberg model with $\theta_{ij} = 0$, and where the perturbation to this Hamiltonian is given by

$$H_1 = \sum_{(i,j)} [\theta_{ij} j_{ij}^{(s)} - \tfrac{1}{4}\theta_{ij}^2 J_{ij}(S_i^+ S_j^- + \text{H.c.})] . \quad (2)$$

Above, $j_{ij}^{(s)} = (i/2)J_{ij}(S_i^+ S_j^- - \text{H.c.})$ is the z component of the spin-current operator. Consider now the case of identical twists, θ_x, that exist only along nearest-neighbor bonds oriented along the x axis. Then since the spin rigidity D_s is related to the difference in the ground-state energy by $E_0(\theta_x) - E_0(0) = ND_s\theta_x^2$ for small θ_x, second-order perturbation theory gives

$$D_s = N^{-1}\left[\frac{1}{2}\langle -T_x^{(s)} \rangle - \sum_{\nu \neq 0} \frac{|\langle 0|j_x^{(s)}|\nu \rangle|^2}{E_\nu - E_0} \right], \quad (3)$$

where the spin kinetic energy operator and the spin-current operator along the x direction are defined by $T_x^{(s)} = \sum_i \tfrac{1}{2}J_{i,i+\hat{x}}(S_i^+ S_{i+\hat{x}}^- + \text{H.c.})$ and $j_x^{(s)} = \sum_i (i/2)J_{i,i+\hat{x}}(S_i^+ S_{i+\hat{x}}^- - \text{H.c.})$, respectively, and where N denotes the number of sites.

We can next consider placing a small uniform dynamical twist, $\theta_x(t) = \theta_x e^{i\omega t}$ on all of the nearest-neighbor bonds that are oriented along the x direction in the modified Heisenberg model (1). Application of the Kubo formula then yields a variation in the ground-state energy per site of $N^{-1}\Delta E_0 = \frac{1}{2}\Pi_{xx}^{(s)}\theta_x^2$, where

$$\Pi_{xx}^{(s)} = N^{-1}\left[\langle -T_x^{(s)} \rangle - \sum_{\nu \neq 0} \left[\frac{|\langle 0|j_x^{(s)}|\nu \rangle|^2}{E_\nu - E_0 - \omega} - \frac{|\langle \nu|j_x^{(s)}|0 \rangle|^2}{E_0 - E_\nu - \omega} \right] \right]. \quad (4)$$

Since the spin current is given by $j_x^{(s)} = \partial E_0/\partial\theta_x = N\Pi_{xx}^{(s)}\theta_x$, the spin conductivity, $\sigma_s(\omega) = \Pi_{xx}^{(s)}/i\omega$, is then just

$$\text{Re}\sigma_s(\omega) = 2\pi\left[D_s\delta(\omega) + N^{-1}\sum_{\nu \neq 0} |\langle 0|j_x^{(s)}|\nu \rangle|^2 \times \delta((E_\nu - E_0)^2 - \omega^2) \right], \quad (5a)$$

$$\mathrm{Im}\,\sigma_s(\omega) = \omega^{-1}\left[\frac{1}{N}\langle -T_x^{(s)}\rangle\right.$$

$$\left. -\frac{2}{N}\sum_{\nu\neq 0}\frac{|\langle 0|j_x^{(s)}|\nu\rangle|^2(E_\nu - E_0)}{(E_\nu - E_0)^2 - \omega^2}\right]. \quad (5b)$$

Integrating Eq. (5a) over all frequencies, and substituting in expression (3) for the spin rigidity, we obtain the following moment sum rule[3] for the spin conductivity:

$$\int_{-\infty}^{\infty} d\omega\,\mathrm{Re}\,\sigma_s(\omega) = \pi\frac{\langle -T_x^{(s)}\rangle}{N}. \quad (6)$$

Hence, the fraction of the moment sum rule occupied by the static twist response is simply

$$I_0 = \frac{\rho_s}{\langle -T_x^{(s)}\rangle/N}, \quad (7)$$

where we define $\rho_s = 2D_s$ to be the spin stiffness. Notice that the above result indicates that the entire magnetic moment is made up only of excited states in unstiff spin systems with $\rho_s = 0$. Below, the spin stiffness, as well as the latter static moment fraction, is computed numerically using the Lanczos technique on finite chains and square lattices for both the ferromagnet and for frustrated antiferromagnets.

Ferromagnet. To check the validity of the method we consider first the nearest-neighbor ferromagnetic spin-$\frac{1}{2}$ chain with periodic boundary conditions. The ground-state of Hamiltonian (1) has been obtained by applying the Lanczos technique for $N = 8, 10, 12, \ldots, 20$ sites in the $S_z = 0$ subspace, that permits introduction of twists along the z axis. After finite-size extrapolation to the thermodynamic limit as function of N^{-1}, we obtain a value for the spin stiffness of $\rho_s/J = 0.248 \pm 0.005$, which is quite close to the exact result of $\rho_s/J = s^2 = \frac{1}{4}$ for spin $s = \frac{1}{2}$.[1] Similar results were obtained in the case of the square lattice. Also, the average spin kinetic energy for the nearest-neighbor ferromagnet is simply the total energy in the $S_z = 0$ subspace; i.e., $\langle T_x^{(s)}\rangle = -Ns^2J$. Hence, Eq. (7) indicates that $I_0 = 1$, which means that the static twist response saturates the moment sum rule (6) in the case of the nearest-neighbor ferromagnet. We have recovered the latter result numerically to within computer accuracy. The saturation effect can also be directly understood by the comparison of expression (3) for the spin rigidity and expression (6) for the moment sum rule, coupled with the observation that the ferromagnetic state is a null eigenstate of the spin-current operator. Hence, the spin response of such a ferromagnet is analogous to the charge-response of noninteracting electrons, where the Drude weight saturates the f sum rule.[1,2]

Frustrated antiferromagnetic chain. Consider next a periodic spin-$\frac{1}{2}$ chain with both nearest-neighbor (J_1) and next-nearest-neighbor (J_2) antiferromagnetic interactions. Again, we have performed exact diagonalizations of Hamiltonian (1) in the $S_z = 0$ subspace for $N = 8, 10, 12, \ldots$, and 20 sites. The stiffness extracted from these studies are shown in Fig. 1. After performing a finite-size extrapolation of our results for the unfrus-
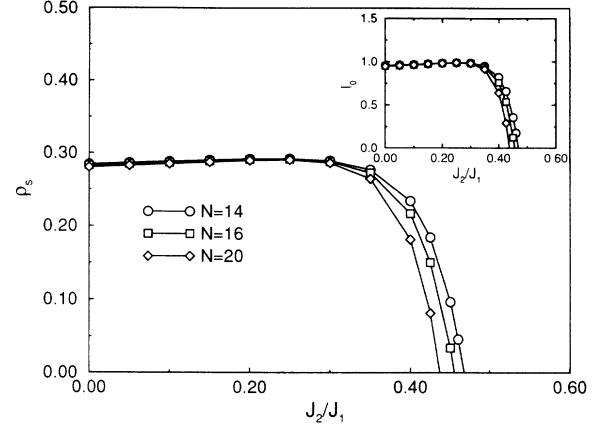

FIG. 1. Shown is the spin stiffness ρ_s of the frustrated antiferromagnetic chain (in units of J_1) as a function of next-nearest-neighbor frustration, J_2/J_1, for various system sizes. The inset displays the fraction, I_0, of the sum rule (6) exhausted by the static twist response.

trated antiferromagnetic chain ($J_2 = 0$) as a function of N^{-1}, we obtain a value of $\rho_s/J_1 = 0.270 \pm 0.005$ for the spin stiffness in the thermodynamic limit, that is slightly greater than the exact value of $\frac{1}{4}$ (see Ref. 1). The small discrepancy we obtain with respect to the exact result could be due to the fact that the existence of *algebraic* long-range order in the spin-$\frac{1}{2}$ Heisenberg chain[1,8] exaggerates finite-size effects.[9] Also, we see from Fig. 1 that while the stiffness rises very slightly upon the introduction of frustration, $J_2 > 0$, it drops precipitously to zero around $J_2/J_1 = 0.43$. This point is in the vicinity of the well studied spin-Peierls dimerization transition,[8] evidenced by the absence of spin rigidity in the chain. Recent estimates that exploit conformal invariance find a value for the latter critical frustration of $J_{2c} \cong 0.24J_1$,[10] which is consistent with the decrease of J_{2c} with increasing lattice size that we observe (see Fig. 1). In fact, finite-size extrapolation of these results yields a value of $J_{2c}/J_1 = 0.33 \pm 0.05$. We have also computed the fraction, I_0, of the moment sum rule occupied by the static twist response, which is shown in the inset to Fig. 1. In the case of the unfrustrated antiferromagnetic chain ($J_2 = 0$), this value extrapolates to $I_0 = 0.915 \pm 0.005$ in the thermodynamic limit, $N^{-1} \to 0$. It is intriguing to remark that the latter value is quite chose to the analogous fraction of the f-sum rule contributed to by the Drude weight in the t-J model chain with one hole,[11] which is 0.938. In addition, this fraction increases to a maximum value approaching unity at $J_2/J_1 \cong 0.25$ of $I_0 = 0.986 \pm 0.005$, just before plummeting to zero.

Frustrated antiferromagnet on the square lattice. We have also diagonalized Hamiltonian (1) for the case of spin-$\frac{1}{2}$ on finite square lattices with nearest-neighbor (J_1), next-nearest-neighbor (J_2), and next-next-nearest-neighbor (J_3) interactions. This model has been widely studied because of its close connection with the t-J model on the square lattice,[12] and hence because of its relation to the phenomenon of high-temperature superconductivi-
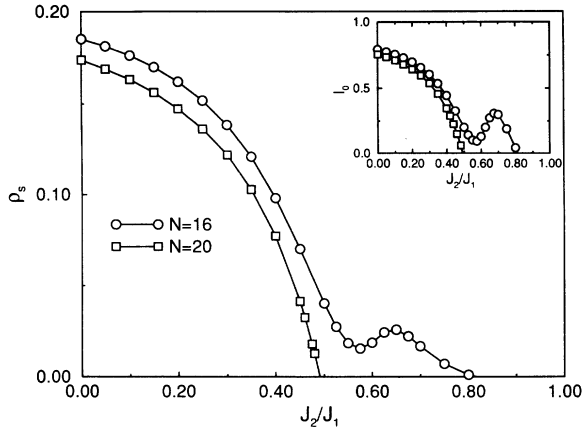
FIG. 2. Above, we display the spin stiffness of the square-lattice Heisenberg antiferromagnet (in units of J_1) with only next-nearest-neighbor (diagonal) frustration, J_2, for various system sizes. The inset shows the corresponding fraction (7) of the moment sum rule exhausted by the static twist response.

FIG. 3. Similar to Fig. 2, with the exception that only next-next-nearest-neighbor frustration, J_3, is considered.

ty.[7,13–15] In particular, we have found ground states for $N = 8, 16, 18$, and 20 site square lattices with periodic boundary conditions[16] via the Lanczos technique. In the case of the nearest-neighbor Heisenberg antiferromagnet we obtain stiffness values of $\rho_s/J_1 = 0.185$, 0.177, and 0.174 for systems sizes of $N = 16, 18$, and 20, respectively. Notice the general downward trend with increasing lattice size. After finite-size extrapolation to the thermodynamic limit we find a value of $\rho_s/J_1 = 0.14 \pm 0.01$. Both this value and the former upper bound of 0.174 for the spin stiffness lie below that of $\rho_s/J_1 = 0.18$ obtained from second-order-spin-wave theory.[5]

Our results for the spin stiffness of the frustrated J_1-J_2 model ($J_3 = 0$) are shown in Fig. 2, while those of the frustrated J_1-J_3 model ($J_2 = 0$) are shown in Fig. 3. As intuitively expected, we observe that the spin stiffness generally decreases smoothly as frustration increases. In particular, the stiffness vanishes near $J_2/J_1 = 0.5$ in the case of the J_1-J_2 model with 20 sites, whereas it vanishes near $J_3/J_1 = 0.35$ in the case of the J_1-J_3 model. The latter parameter values are close to the points where the corresponding classical model loses its long-range Néel order.[7] The fraction, I_0, of the moment sum rule exhausted by the static twist response for both the J_1-J_2 and the J_1-J_3 models are also plotted in the insets of Fig. 2 and 3, respectively. Figure 2 shows that the J_1-J_2 model on the 4×4 lattice has a distinct feature near its classical critical point for values of frustration ranging from $J_2/J_1 \cong 0.55$ to $J_2/J_1 \cong 0.80$. Here, the spin stiffness rises with increasing frustration, but then finally vanishes.
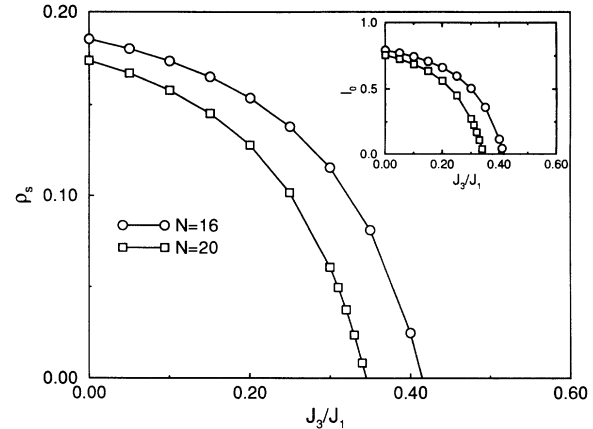
It has been pointed out in the literature that uniform chiral correlations peak near this region,[14] and that the excited states in this vicinity are spin singlets.[15] This feature could therefore correspond to a phase with uniform chiral spin order,[13] since the latter state is characterized by spin-0 excitations. A spin-glass phase, however, is not ruled out.[15] Note that the absence of this feature on the other 18 and 20 site lattices that we have studied could be due to their "tilted" nature.[16] For example. collinear order—which we know must occur in the thermodynamic limit for large values J_2[7]—is not possible in such lattices. Clearly, similar diagonalizations of Hamiltonian (1) on a 6×6 lattice are necessary in order to resolve this issue.

In summary, we have extended the theory of the determination of spin rigidity via twisted boundary conditions[1] to the general case of quantum Heisenberg models. This method has been applied for the first time to the exact diagonalization of frustrated spin-$\frac{1}{2}$ antiferromagnetic chains and square lattices. Notably, we find an upper bound of 0.174 for the spin stiffness of the unfrustrated antiferromagnetic Heisenberg model on the square lattice that agrees to within a few percent with spin-wave calculations.[5] However, the extrapolated value of 0.14 ± 0.01 obtained from finite-size scaling to the thermodynamic limit is considerably smaller.

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