Anomalous Finite Size Spectrum in the $S = 1/2$ Two Dimensional Heisenberg Model

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We study the low energy spectrum of the nearest neighbor Heisenberg model on a square lattice as a function of the total spin S. By quantum Monte Carlo simulation we compute this spectrum for Heisenberg models with local moments $s = 1/2$, $s = 1$, and $s = 3/2$. We conclude that the nonlinear σ model prediction for the low energy spectrum is always verified for a large enough system size. However, the crossover to the correct scaling regime is particularly slow just for the $s = 1/2$ Heisenberg model. The possible detection of this unexpected anomaly with finite temperature experiments on $s = 1/2$ isotropic quantum antiferromagnets is also discussed. [S0031-9007(98)05396-4]

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The square lattice Heisenberg model (HM) has attracted much attention in recent years because of its connection with the antiferromagnetic properties of the undoped stoichiometric compounds of high-T_c superconductors [1]. The model Hamiltonian in general dimension d reads

$$H = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j \,, \tag{1}$$

where the symbol $\langle i, j \rangle$ indicates nearest neighbor summations, the index i labels the positions R_i of the $N = L^d$ sites on a hypercubic lattice, and the quantum spin operators satisfy $(\vec{S}_i)^2 = s(s + 1)$. What makes particularly difficult any analytical treatment of this model is the fact that the antiferromagnetic order parameter $\vec{m} = \frac{1}{N} \sum_i e^{iQR_i} \vec{S}_i$ [with $Q = (\pi, \pi, ...)$] does not commute either with the Hamiltonian or with the total spin $S = \sum_i \vec{S}_i$. Whenever long range order is present in the thermodynamic limit, a huge degeneracy of the energy spectrum $E(S)$ as a function of the total spin S is implied by the mentioned noncommutativity. Hence $E(S)$, referenced to the singlet $S = 0$ ground state energy, is predicted to behave as the spectrum of a free quantum rotator as long as $S \ll \sqrt{N}$ [2–5],

$$E(S) = S(S + 1)/2IN \,, \tag{2}$$

where I is known as the *momentum of inertia* per site.

This equation resembles the definition of the spin susceptibility χ which is, however, obtained by taking *first* the infinite volume limit of the energy per site $e(m) = E(S)/N$ at fixed magnetization $m = S/N$ and then letting $m \to 0$: $e(m) = m^2/(2\chi) + o(m^2)$. An identification between I and χ is possible only if the excitation spectrum smoothly connects the low energy portion, which corresponds to total spin $S \sim O(1)$, with the regime of macroscopic spin excitations: $S \sim mN$ (with $m \ll 1$). This is a highly nontrivial statement which is actually verified by the underlying low energy model of the quantum antiferromagnet (QAF), known as the nonlinear σ model (NLσM) [4–6].

For the HM in one dimension the accepted low energy model is instead the Luttinger liquid with $K_\sigma = 1/2$, and the prediction in this case is that the energy spectrum as a function of the total spin behaves as $E(S) = S^2/2\chi N$ where χ coincides with the spin susceptibility [7]. Note the strong analogy of the spectrum in one and higher dimensions, although in the former case no true long range order sets in.

It is particularly important to verify that, also in the presence of long range order, the low energy spectrum of the microscopic Hamiltonian conforms to the prediction of the low energy effective model. This is the main problem addressed in this paper where we show the results of high accuracy computations of the energy spectrum $E(S)$ in a few two dimensional nonfrustrated spin models. To this purpose we use an improved version of the known lattice Green's function Monte Carlo (GFMC) technique introduced some years ago by Trivedi and Ceperley [8]. Our method allows us to control any form of systematic error in a rigorous and simple way [9]. For large lattice size, the energy difference between spin subspaces becomes extremely small. Nevertheless, our technique allows a good resolution of the spectrum $E(S)$ up to a 16×16 lattice with a reasonable computational effort. The method we use allows us to eliminate exactly any source of systematic error which affects previous GFMC calculations [10]. For large size the results by Runge are also affected by a non-negligible population control error which is exactly eliminated in this GFMC scheme [9]. Our results for the ground state energy are instead consistent with those shown in Ref. [11], obtained with a completely different QMC method [12].

If the quantum top law (2) is verified, we can calculate the unknown quantity $1/2\chi$ on a finite lattice by inserting the computed excitation energies at different spin S in the equation

$$[2\chi_S]^{-1} = N\,E(S)\,[S(S + 1)]^{-1}. \tag{3}$$

Clearly, $1/\chi_S$ should approach the physical inverse susceptibility for infinite size and for any spin excitation $S \ll N$ provided the quantum top law is verified.

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It is then instructive to study the deviations from Eq. (2) through the quantity

$$\Delta\chi^{-1} = \left[\frac{1}{2\chi_S} - \frac{1}{2\chi_L}\right] S(S+1), \tag{4}$$

which is zero for $S = 0$ and $S = L \ll N$, by definition, and should vanish for any fixed S in the $N \to \infty$ limit. A finite slope in the numerical data, as clearly shown by Fig. 1 for $s = 1/2$, would imply $1/2I > 1/2\chi_L$, with a violation of the quantum top law. A similar, and even more pronounced, anomaly was also reported in Ref. [13] to support the existence of a spin liquid phase for the spatially anisotropic HM with strong anisotropy. Figure 1 provides clear evidence that this anomaly in the spectrum surprisingly persists in the isotropic 2D HM for $s = 1/2$ HM while it is absent, within statistical errors, in the higher spin models shown in the same figure. This apparently contrasts with the accepted picture stating that the low energy properties of the $s = 1/2$ HM can be fully described by the NLσM.

How can we reconcile this numerical evidence with the established theories of the 2D $s = 1/2$ quantum antiferromagnets? Does this anomaly have an observable consequence in the low energy behavior of the 2D HM? In order to answer these questions, it is important to have a better control of the finite size corrections, because the data presented in this paper are close to the limits of the available computers and a considerably larger size cannot be handled with the required accuracy.

In the following, we will make extensive use of spin wave theory (SWT) [2,14] which is known to be extremely accurate for the HM. For instance, the recent quantum Monte Carlo (QMC) calculation of the order parameter gives $m \simeq 0.31$ [9–11], quite close to the linear spin wave (SW) estimate $m \simeq 0.3$. Moreover, SWT, which is based on a systematic expansion in $1/s$, can be generalized without basic difficulties to finite systems, making possible a direct comparison of the numerical results with the spin wave predictions [15].

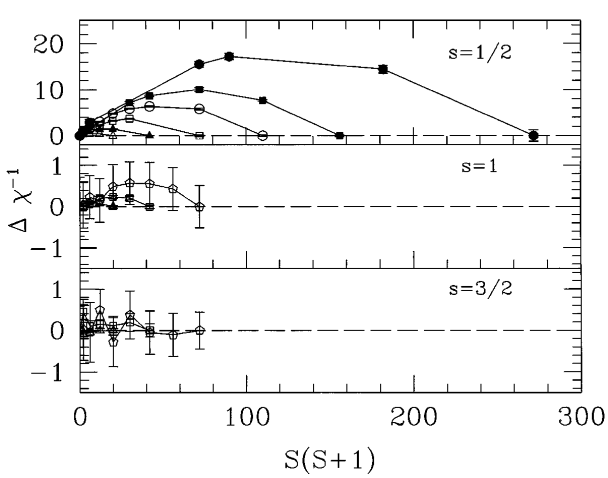

FIG. 1. $\Delta\chi^{-1}$ for 2D HM of spin $s = 1/2$ (data up to $N = 256$), $s = 1$ (data up to $N = 100$), and $s = 3/2$ (data up to $N = 64$). Lines are guides to the eye.

In order to study the spin excitation spectrum of the model as a function of the total spin, we add to the HM Hamiltonian H a magnetic field along the z direction: $H_h = H - hs\sum S_i^z$. The magnetic field h can be chosen to stabilize the desired spin excitation of spin S. In order to perform a systematic SW calculation for large s, we have scaled the magnetic field by s. In this way, when $s \to \infty$ the magnetic energy due to the external field $hs\sum S_i^z$ is of the same order $\sim s^2$ as the average energy $E(S) = \langle H \rangle$. The classical solution for $s \to \infty$ at fixed h is simply obtained by canting the spins of an angle θ in the direction of the field (with $\sin\theta = \frac{h}{4d}$). By the use of the standard Holstein-Primakoff representation of the spin operators in terms of bosons and by expanding the resulting Hamiltonian in powers of $1/s$, we can compute the fluctuations over the classical solution and obtain the linear SW estimate of the energy of H_h [15,16],

$$\begin{aligned} E(h) &= -Js^2N(d - h^2/8d) - Jds\left(N - \sum_k \epsilon_k\right), \\ \epsilon_k &= \tfrac{1}{4d}\left[16d^2(1-\gamma_k^2) - 2h^2\gamma_k(1-\gamma_k)\right]^{1/2}, \end{aligned} \tag{5}$$

with $\gamma_k = (\cos k_x + \cos k_y + \ldots)/d$. By expanding $E(h)$ about $h = 0$, we get $E(h) \sim -\frac{1}{2}\chi^{\mathrm{SW}}(sh)^2$ which immediately gives the well known linear SW correction to the classical spin susceptibility $\chi_0 = 1/4dJ$: $\chi_{\mathrm{SW}}/\chi_0 = 1 - 0.55115/2s$ [14]. This calculation can be extended to the next leading order and gives the second order correction to χ,

$$Z_\chi = \chi/\chi_0 = 1 - 0.55115/2s + 0.0403/(2s)^2. \tag{6}$$

After a careful treatment of the umklapp processes our expansion coincides with the one obtained before by Igarashi and Watabe [17] with a different approach. Later publications instead reported contradictory results about the expansion (6) [18].

The energy spectrum $E(S)$ of the $s = 1/2$ HM as a function of the total spin S can be evaluated within linear SWT in two equivalent ways. We can either perform the Legendre transform $E(S) = E(h) + hsS$ of Eq. (5) at fixed $s = 1/2$ (referred to as SWH), or we can scale the spin $S = \mu s$ with fixed μ evaluating the Legendre transformed $E(\mu s)$ perturbatively in $1/s$ before setting $s = 1/2$ (referred to as SWM). Of course, these two methods are equivalent within a $1/s$ expansion, and the differences only arise because we truncate SW expansion at a finite order in $1/s$. The apparent deviations from the quantum top law shown in Fig. 1 can be understood on the basis of the aforementioned linear SW analysis. To this purpose, in Fig. 2 we compare the SWH prediction for $1/2\chi_L - 1/2\chi_{L/2}$ with the QMC data.

We see that both QMC and SWH results, although quantitatively different, show the same dependence on lattice size with an apparent plateau at about $L \sim 10$ which would suggest a breakdown of the quantum top

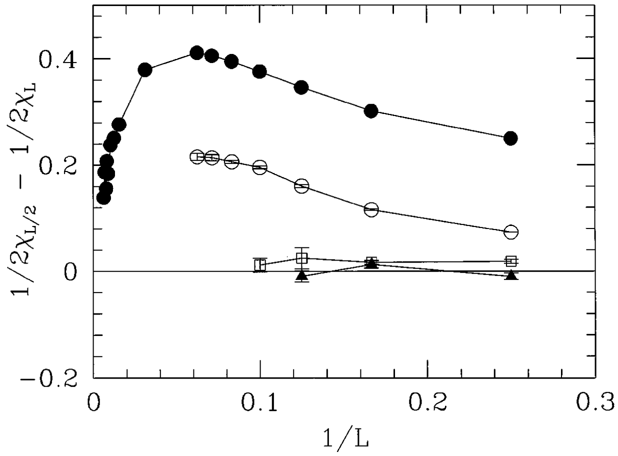

FIG. 2. Size dependence of $1/2\chi_S$ as defined in (3) for the 2D HM. Upper curve: linear spin wave. QMC data refer to $s = 1/2$ (circles), $s = 1$ (squares), and $s = 3/2$ (triangles). Lines are guides to the eye.

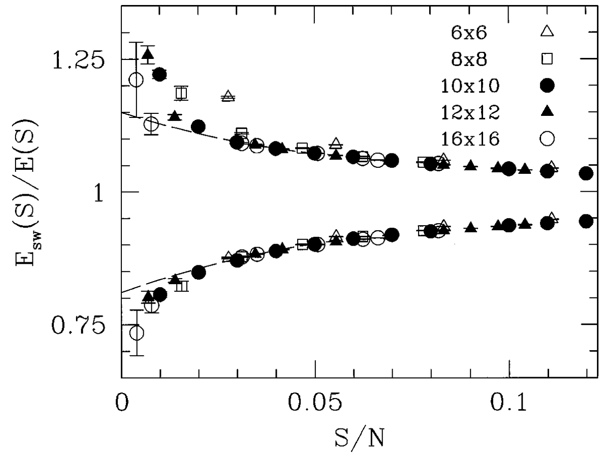

FIG. 3. Ratio of the QMC spectrum with linear SWM (lower curve) and SWH (upper curve) for several system sizes. The curves are least squares fits of the data.

law. While QMC data stop because it is not possible to obtain high quality data at larger size, the SW results show an abrupt change of behavior with a clear convergence towards the expected result. The correct $1/L$ scaling is, however, reached for only $L > 32$.

The similarity between QMC and SWH, where both available, suggests that the nonmonotonic behavior is a genuine feature of the model. In order to provide support for this scenario, we considerably reduced the anomalously large finite size corrections present in Fig. 2 by taking the ratio between the energy spectrum evaluated via QMC and SWT (using both the SWM and SWH methods). As shown in Fig. 3 we get a remarkable collapse of all the QMC data for sufficiently large sizes ($L \sim 10-16$) onto a single curve, even at small total spin S. This is a direct confirmation that the anomalies detected in the spectrum of the $s = 1/2$ HM are quite similar to those present in linear SWT, and eventually disappear only for very large size. We stress that this unexpected behavior is visible only in the $s = 1/2$ HM and is strongly reduced for higher s (but also in spin-anisotropic systems like the XY model). This suggests that quantum fluctuations, enhanced by small values of s, deeply affect the properties of the model when the spontaneous breaking of a non-Abelian symmetry occurs.

We also notice that at small spin excitations the size effects are not so dramatic as shown in Fig. 4(a) where the QMC ratio $E(S = 2)/E(S = 1)$ is seen to smoothly approach the value 3 predicted by the quantum top law (dashed line). The possibility to control the anomalously large finite size effects allows for an accurate numerical estimate of the spin susceptibility even in the $s = 1/2$ HM. In fact, the susceptibility can be directly obtained by extrapolating to zero magnetization $m = S/N$ the QMC results shown in Fig. 3. However, only data representative of the thermodynamic limit of the energy per site $e(m) = E(S)/N$ must be included in the extrapolation procedure. As shown in Fig. 3 the QMC ratios to both SWH and SWM predictions can be nicely extrapolated to $m = 0$ if we exclude points with $m < 0.03$. On the other hand, the thermodynamic limit of the SW results can be obtained analytically: $e(m) = m^2[2\chi_0(1 - 0.55115/2s)]^{-1}$ and $e(m) = m^2[2\chi_0]^{-1}(1 + 0.55115/2s)$ for the SWH and SWM estimate, respectively. Both methods consistently give the following result for the spin susceptibility of the $s = 1/2$ HM:

$$Z_\chi = \chi/\chi_0 = 0.523 \pm 0.005 \,. \tag{7}$$

Our value for Z_χ is also consistent, within error bars, with the independent calculation of I shown in Fig. 4(b) and is not far from the second order SW value (6). This result slightly differs from series expansion Ref. [19] but much more from previous finite size scaling analysis based on QMC data on similar lattice sizes [10,11].

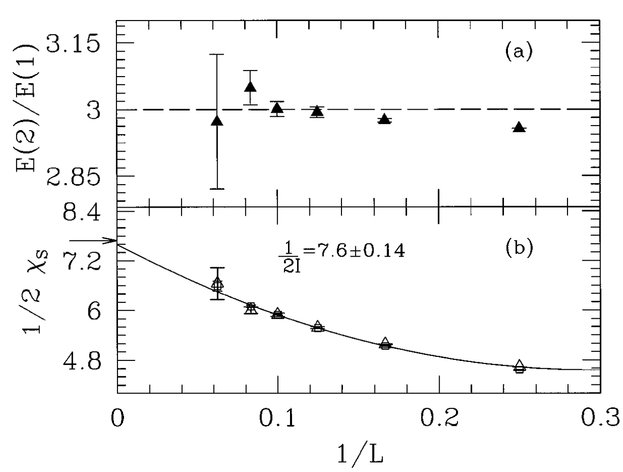

FIG. 4. (a) Ratio between the $S = 2$ and $S = 1$ excitation energies. (b) Size dependence of $1/2\chi_S$ (3) for $S = 1$ (triangles) and $S = 2$ (squares). The arrow shows the expected $1/2\chi$ (see Fig. 3). The continuous line is a parabolic extrapolation ($1/2I = 1/2\chi_S$ for $L \to \infty$) for $S = 2$ and $6 \leq L \leq 16$.

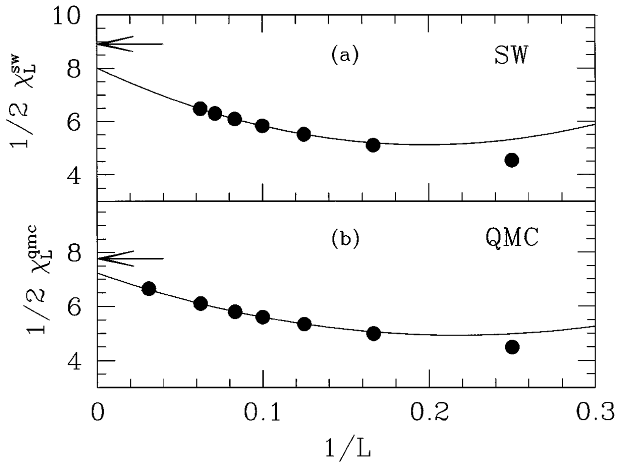

FIG. 5. Same as Fig. 4(b) for the spin excitation $S = L$. Curves are parabolic extrapolations. The arrows are the expected infinite size limits.

The latter discrepancy can easily be understood on the basis of the strong finite size anomaly in the spectrum of the $s = 1/2$ HM we have discussed. In fact, as shown in Fig. 5(a) if we extrapolate to the thermodynamic limit the known SW spectrum in lattices with $L < 16$ by use of the correct asymptotic scaling $\chi_L = \chi_\infty + a/L + b/L^2$ [3–5], we get a poor estimate of the exact $L \to \infty$ limit of χ_{SW}. In fact, SWT suggests that the correct scaling is valid only for extremely large sizes ($L > 64$), while it is not accurate for the lattice sizes where QMC simulations are available [see Fig. 5(b)].

A further evidence that the data shown in Fig. 3 are very weakly size dependent comes from the consistency with the NLσM next leading $m \to 0$ prediction [4] for $e(m) = (1/2\chi)m^2 - (1/12\pi c^2\chi^3)m^3$. This allows one to determine from the slopes for $m \to 0$ in Fig. 3 the SW velocity $c/c_0 = 1.18(4)$ (upper curve), $c/c_0 = 1.1(10)$ (lower curve) in good agreement with the expectations [8–11].

In conclusion, we have given convincing evidence that the low energy spectrum of the 2D quantum antiferromagnet is consistent with the prediction of the $(2 + 1)$D-NLσM. Unexpected anomalies in the finite size spectrum are, however, detected in the $s = 1/2$ HM. The physical origin of these size corrections can be understood on the basis of linear SW approximation: One of the two gapless excitations present in the SU(2) model acquires a mass when an external magnetic field is applied. The competition between the massive and the massless modes becomes quite strong in the $m \to 0$ limit leading to the observed anomalies. Making use of the results of SWT, we have been able to obtain a very accurate estimate for the spin susceptibility.

This extensive discussion of finite size effects in the low energy spectrum of the 2D HM has interesting connections with the finite temperature behavior of the system. In fact, on the basis of the mapping to the NLσM, the properties of the HM at finite temperature T coincide with those at $T = 0$ of a HM in an infinitely long strip of width $L = 1/T$ and periodic boundary conditions. By applying the finite size SW analysis to the stripe geometry, we then evaluate the uniform magnetization m in an external magnetic field h at temperature T,

$$m(h,T) = \chi h + \frac{h^2}{4\pi c^2} + \frac{hT}{2\pi c^2}\ln(1 - e^{-h/T}). \quad (8)$$

This expression, asymptotically valid for small h and T but arbitrary ratio h/T, obeys the known scaling form predicted by Fisher [4,5]. The anomalous finite size corrections in the energy spectrum we have uncovered also suggest the possible presence of a *small* crossover temperature $T_\times$ corresponding to the maximum in Fig. 2. In the HM, $k_B T_\times$ can be estimated as a few percents of the natural energy scale J. The observable consequences of this possible anomalous behavior of the low temperature susceptibility of the 2D HM should be reconsidered on the basis of this study.

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