# Two-Dimensional Spin-$\frac{1}{2}$ Antiferromagnetic Heisenberg Model versus Nonlinear $\sigma$ Model

Efstratios Manousakis[(1)] and Román Salvador[(2)]

[(1)]Department of Physics, Center for Materials Research and Technology, and Supercomputer Computations Research Institute, Florida State University, Tallahassee, Florida 32306

[(2)]Control Data Corporation and Supercomputer Computations Research Institute, Florida State University, Tallahassee, Florida 32306

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We study the continuum limit of the nonlinear $\sigma$ model in 2+1 dimensions and at finite temperature $T$, using Monte Carlo simulation on large lattices. Even though the lattice spacing vanishes, *dimensional transmutation* occurs which makes the correlation lengths finite. *Assuming* that the $\sigma$ model and the spin-$\frac{1}{2}$ antiferromagnetic Heisenberg model are equivalent at low $T$, we make contact between the two models and find that the latter model must order at $T=0$. Our results are consistent with neutron-scattering experiments done on $La_2CuO_4$.

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The discovery of the copper-oxide superconductors, as well as the suggestion that the superconductivity mechanism in these new materials is related to the strong correlations among purely electronic degrees of freedom,[1] has intensified the interest for understanding one of the simplest models to account for such correlations: the Hubbard model. The strong two-dimensional (2D) spin correlations observed in neutron-scattering experiments[2] have given credit to the spin-$\frac{1}{2}$ antiferromagnetic (AF) Heisenberg model defined as

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

where $\mathbf{S}_i$ is the spin-$\frac{1}{2}$ operator of the conduction-band electrons localized in the Wannier states around the $i$th unit cell of the copper-oxide plane. $J$ is the AF coupling and the sum is over the nearest neighbors. This model can be obtained from the Hubbard model at half filling by taking the strong-coupling limit.[3] In such a formulation, the Heisenberg model describes interactions that originate from virtual electron hopping processes.

Recently we simulated[4,5] the spin-$\frac{1}{2}$ 2D AF Heisenberg model using Handscomb's quantum Monte Carlo (MC) method. We calculated the correlation length and found that it increases very rapidly with decreasing temperature. The results of Refs. 4 and 5 are consistent with neutron-scattering experiments. It is, however, difficult to find an efficient quantum MC algorithm to study large systems and approach low temperatures.

The 2D quantum Heisenberg model is believed to be equivalent[6] to the nonlinear $\sigma$ model in the two space plus one Elucidean time dimensions and at low temperatures. More recently, however, there was a suggestion[7] that in the derivation of the nonlinear $\sigma$ model from the Heisenberg model one encounters a topological term. This term distinguishes the integer from the half-integer spin case. The role which such topological terms might play in the development of the theory of superconductivity in the copper oxides was part of the reason for the excitement about this idea. Later, however, the necessity of such topological terms became less clear and in fact, today, the two models are believed to be equivalent without any additional terms.[8]

The nonlinear $\sigma$ model in 2+1 dimensions has been recently studied by Chakavarty, Halperin, and Nelson (CHN).[9] Using a one-loop perturbative renormalization-group approach, CHN relate the nonlinear $\sigma$ model to the spin-$\frac{1}{2}$ Heisenberg AF model at low temperatures and give a good fit to the data obtained from neutron-scattering experiments done on $La_2CuO_4$.

In this paper we study the nonlinear $\sigma$ model in two space plus one Euclidean time dimensions and at finite physical temperature using the MC method. The simulation of this model is easier than that of the quantum AF Heisenberg model. Using efficient vectorized algorithms suitable for ETA supercomputers we study large-size lattices ($100\times100\times8$ is our largest lattice). We calculate the model's renormalization-group $\beta$ function around the 3D critical point which separates the quantum disordered phase from the phase with spontaneous symmetry breaking. Using the $\beta$ function, we rescale the calculated correlation lengths at various values of the coupling $g$ and temperature $T$ and find that all collapse on the same curve independent of $g$ and the lattice spacing. This gives rise to *dimensional transmutation*, a phenomenon well known in field theory, which produces a finite length scale. Assuming that the spin-$\frac{1}{2}$ AF Heisenberg model and the $\sigma$ model are equivalent at low temperatures, we make contact between the two models by comparing the behavior of the correlation lengths at low temperatures. We find that the two models can be made equivalent if the spin-$\frac{1}{2}$ AF Heisenberg model orders at $T=0$. We obtain a reasonable fit to the neutron-scattering data[2] of the insulator $La_2CuO_4$ by taking $J=1270$ K, a value close to that reported by Raman scattering experiments.[10]

The nonlinear $\sigma$ model in two space plus one Euclidean time dimensions is defined as[6,9]

$$S_{\rm eff}=\frac{\rho_0}{2\hbar c}\int_0^{\beta\hbar c}d\tau\int dx\,dy[(\partial_x\mathbf{\Omega})^2+(\partial_y\mathbf{\Omega})^2+(\partial_\tau\mathbf{\Omega})^2]\,. \quad (2)$$

Here $\mathbf{\Omega}$ is a three-component vector field living on a unit sphere, $c$ is the spin-wave velocity, and $\beta=1/k_BT$. We discretize the space-time and put the model on the (2+1)-dimensional lattice:

$$S_{\rm eff}=-\frac{1}{2g}\sum_{\mathbf{x}}\sum_{\mu=1}^{3}\mathbf{\Omega}(\mathbf{x})\cdot[\mathbf{\Omega}(\mathbf{x}+\hat{\mathbf{e}}_\mu)+\mathbf{\Omega}(\mathbf{x}-\hat{\mathbf{e}}_\mu)]\,, \quad (3)$$

where $g=\hbar c/\rho_0 a$, $\mathbf{x}$ covers the (2+1)-dimensional lattice of lattice spacing $a$, size $N^2N_\beta$, and

$$\beta\hbar c=N_\beta a\,. \quad (4)$$

We have to impose periodic boundary conditions (BC) in the Euclidean time direction. In this model the average of the field $\mathbf{\Omega}$ is proportional to the average staggered magnetization and could describe the dynamics of the spins within one isolated $CuO_2$ layer.

From the two-point function we can calculate the correlation length in lattice units $\xi_{\rm latt}$ as a function of $g$, $N_\beta$, and $N$. For continuum-limit behavior and for eliminating finite-size effects, $\xi_{\rm latt}$ must satisfy $1\ll\xi_{\rm latt}\ll N$. We need to take the limit $N\to\infty$ and keep the time dimension finite so that Eq. (4) is satisfied. If, therefore, $N$ is large enough so that $\xi_{\rm latt}\ll N$, the correlation length is only a function of $N_\beta$ and $g$. In physical units $\xi$ is given by

$$\xi=\xi_{\rm latt}(g,N_\beta)a\,. \quad (5)$$

In our simulation we used periodic BC in the space boundaries also. We used the heat-bath algorithm and typically 5000 MC steps over the entire lattice for thermalization and about 10000 for measurements. The correlation length is extracted from the correlation function $G(x_1-x_1')$ of the (Euclidean) time average of $\mathbf{\Omega}(\mathbf{x})$ at two different points in space $x_1$ and $x_1'$. We fitted the long-distance behavior of the correlation function with $A\cosh[(x_1-x_1'-N/2)/\xi_{\rm latt}]$. It is known that for $g>g_c$, where $g_c$ is the 3D critical point (i.e., at $T=0$), the three modes of the theory have degenerate finite masses (inverse correlation lengths). For $g<g_c$, however, there are two masses in the theory: Two modes correspond to the Goldstone-mode excitations and become massless in the 3D theory ($\beta\to\infty$). They are related to the radial motion of the average field and give an exponentially small mass with the size of the finite $\beta$. There is also a massive mode associated with fluctuations in the magnitude (radial component) of the average field. In this paper we study the mode having the smallest mass, which dominates the behavior of the correlation function at large distances.

Keeping the physical temperature constant we may approach the continuum limit $a=\hbar c\beta/N_\beta\to 0$ by increasing $N_\beta$. To keep the correlation length $\xi$ constant in physical units, for any $a\to 0$, we should find the value of $g$ which gives the same value of $\xi$. This is achieved through Eq. (6) which defines the function $g(a)$. The combination of Eqs. (4) and (5) gives $\xi=b\hbar c/k_BT$, where $b=\xi_{\rm latt}(g,N_\beta)/N_\beta$. In order to keep $\xi$ constant at a fixed temperature we should keep the ratio $b$ constant. $b$ is the physical value of the correlation length at temperature $T$ in units of $a_T\equiv\hbar c/k_BT$. In Fig. 1 we give $b$ as a function of $g$ for several values of $N_\beta$. We notice that the lines for various $N_\beta$ pass through the same point $(g_c,b^*)=(1.45\pm0.01,0.80\pm0.05)$. Let us say that we would like to define the theory's coupling constant at the value $b=b_0$ shown in Fig. 1. The line $b=b_0$ intersects the various curves for different $N_\beta$'s (i.e., in this case in which the temperature is constant, for different $a$'s), and the values of $g$ at the intersections define $g(a_T/N_\beta)$. We note that $\lim_{N_\beta\to\infty}g(a_T/N_\beta)=g_c$. Because $b=b^*$ at $g=g_c$, for large $N_\beta$'s (small $a$'s) we obtain

$$\xi^*=b^*\hbar c/k_BT\,, \quad (6)$$

where $b^*=0.80\pm0.05$. Notice that at $T=0$, $g_c$ turns into a critical point. These results confirm the crossover phase diagram given by CHN on general grounds (Ref. 9). Moreover, in their more recent work (Ref. 11), they obtain for the universal constant $b^*=1.1$, a value somewhat higher than ours.

Using our results for the correlation length obtained on lattices of sizes $50^2\times N_\beta$ and $100^2\times N_\beta$ with $N_\beta=2$, 4, 6, and 8, we calculate the renormalization-group $\beta$ function $\beta_{\rm RG}\equiv-a\,dg(a)/da$. Our results for $\beta_{\rm RG}$ are shown as the inset in Fig. 1. To avoid finite-size effects we used only those points for which $b<2.5$. At $g=g_c$, $\beta_{\rm RG}$ changes sign. At $T=0$, $\xi^*=\infty$, and for $g<g_c$ the system enters a phase with spontaneous symmetry breaking, where the staggered magnetization is nonzero. We see that close to the critical point $\beta_{\rm RG}(g)$ is linear:

$$\beta_{\rm RG}(g)=-\beta_1(g-g_c)+\ldots\,. \quad (7)$$

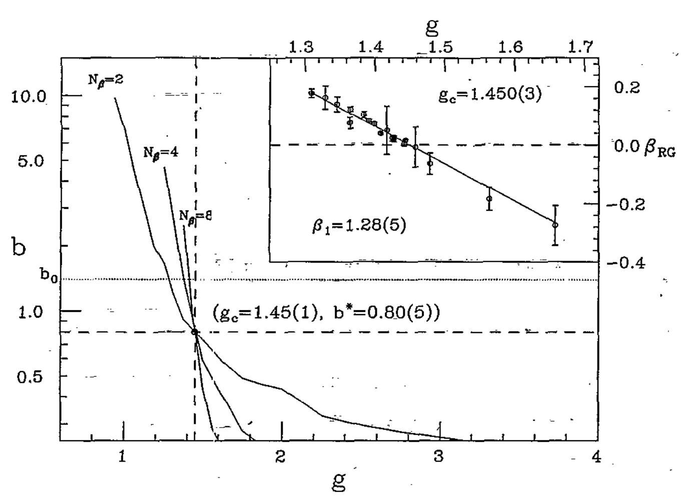


FIG. 1. The ratio $b=\xi_{\rm latt}/N_\beta$ vs $g$ for different $N_\beta$. Notice that all the lines for different $N_\beta$ pass through the same (fixed) point $(g_c,b^*)$. Inset: The renormalization-group $\beta$ function.

We find $g_c = 1.450 \pm 0.003$ and $\beta_1 = 1.28 \pm 0.05$. Integrating both sides of the equation defining $\beta_{\rm RG}$ one obtains $a(g) = a_\sigma \exp[-\int^g dg/\beta_{\rm RG}(g)]$, where $a_\sigma$ is a constant of integration having dimensions of length. The above equation defines the function $g(a)$ which characterizes the continuum theory. $a_\sigma$ is a characteristic parameter of the theory and the cutoff should be removed in a way such that $a_\sigma$ remains constant. In field theory, this limiting process where a vanishing length scale ($a \to 0$) and a dimensionless parameter ($g$) produce a dimensional quantity ($a_\sigma$) is called *dimensional transmutation.*[12]

We have compared our numerical results with results obtained in the saddle-point approximation. We find good agreement in the region $g > g_c$, but poor agreement for $g < g_c$. The saddle-point approximation and details of the present calculation will be given elsewhere.[13]

Using the linear approximation [Eq. (7)] close to the critical point we find

$$a(g) = a_\sigma |g - g_c|^{1/\beta_1}. \tag{8}$$

Combining Eqs. (4) and (8) we obtain

$$N_\beta = |g - g_c|^{-1/\beta_1} T_\sigma / T, \tag{9}$$

where $k_B T_\sigma = \hbar c / a_\sigma$. Substituting $a(g)$ and $N_\beta$ from Eqs. (8) and (9) into Eq. (5) we obtain

$$\frac{\xi}{a_\sigma} = f\left(\frac{T}{T_\sigma}\right) \equiv \xi_{\rm latt}\left(g, |g - g_c|^{-1/\beta_1} \frac{T_\sigma}{T}\right) |g - g_c|^{1/\beta_1}. \tag{10}$$

Since the constants $a_\sigma$ and $T_\sigma$ are independent of $g$ and $a$ and $\xi$ is also independent of $g$ in the process of removing the cutoff, the function in Eq. (10) is only a function of $t \equiv T/T_\sigma$. In Fig. 2 we show the function $f(t)$. The data points in the figure correspond to various $g < g_c$ and $N_\beta$ values. We see that all scale to a universal curve. Again, we emphasize the occurrence of dimensional transmutation where, although the lattice spacing is removed together with $g$, we obtain correlation lengths in units of a finite length scale $a_\sigma$ as a function of temperature $t$ in units of $T_\sigma$.

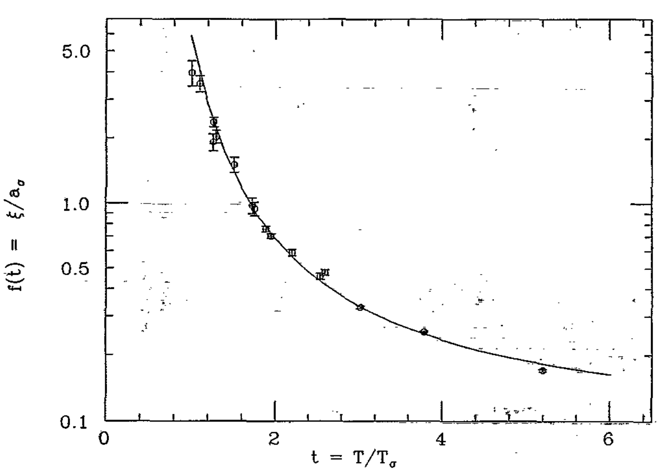


FIG. 2. The function $f(t)$ (see text for definition). Our data for various $g$'s collapse on the same curve by using the calculated renormalization-group $\beta$ function. The solid line corresponds to an exponential fit [Eq. (11)].

The curve $f(t)$ can be approximated by an exponential,

$$f(t) = A_\sigma \exp(B_\sigma / t), \tag{11}$$

as the saddle-point approximation (Ref. 13) and the most recent work of CHN (Ref. 11) suggest. The best fit gives $A_\sigma = 0.0795$ and $B_\sigma = 4.308$, and is shown as a solid line in Fig. 2.

For $g \gg g_c$ the correlation length in the nonlinear $\sigma$ model is only a function of $g$ and is independent of $T$. At the critical point $g = g_c$ we find that at low $T$, $\xi$ grows as $1/T$ as the temperature decreases.

It is possible to make contact between the spin-$\frac{1}{2}$ AF Heisenberg model and the nonlinear $\sigma$ model. In Refs. 4 and 5 we simulated the former and we found it to grow much more rapidly than $1/T$. More precisely, in Ref. 4, we fitted the correlation lengths by $\xi(T) = C/Te^{b/T}$, as suggested by the spin-wave theory, and by the Kosterlitz-Thouless form $\xi(T) = Ce^{b/|T-T_c|^{1/2}}$. We found that the latter form fits better and concluded that our simulation indicated that topological excitations may play an important role in the dynamics of the spin-$\frac{1}{2}$ Heisenberg antiferromagnet. Following our findings for the $\sigma$ model we attempt to fit our numerical results for the Heisenberg model by

$$\xi / a_H = A_H \exp(B_H J / T). \tag{12}$$

This form, i.e., without the $1/T$ prefactor, also fits our data well, giving $A_H = 0.25$ and $B_H = 1.4$ (Ref. 5, Table II). On this basis we may conclude that if data do not exist at very low temperatures, prefactors may play an important role. Hence the results of our simulation[4,5] may also be consistent with spin-wave theory and the existence of an ordered state at $T = 0$.

Let us *assume* that the two models are equivalent at low $T$. In order to obtain the best fit between the correlation lengths calculated for the two models, we need to assume that the spin-$\frac{1}{2}$ AF Heisenberg model corresponds to the broken phase ($g < g_c$) of the $\sigma$ model in the continuum limit. Therefore the spin-$\frac{1}{2}$ AF Heisenberg model should order at $T = 0$ and $A_H a_H = A_\sigma a_\sigma$ and $B_H J = B_\sigma T_\sigma$. We obtain $a_\sigma = 3.14 a_H$ and $\hbar c \simeq 1.02 J a_H$. In Oguchi's calculation,[14] the value of the renormalized spin-wave velocity for a spin-$\frac{1}{2}$ antiferromagnet $\hbar c = 1.64 J a_H$ is lower than our value for the bare spin-wave velocity which enters in the nonlinear $\sigma$ model. More recently Gomez-Santos, Joannopoulos, and Negele (GJN)[15] have performed similar simulations of the spin-$\frac{1}{2}$ AF Heisenberg model. They find overall agreement at higher temperatures with our results reported in Ref. 4, but they find some 20% smaller correlation lengths at lower temperatures. GJN argue that the ori-

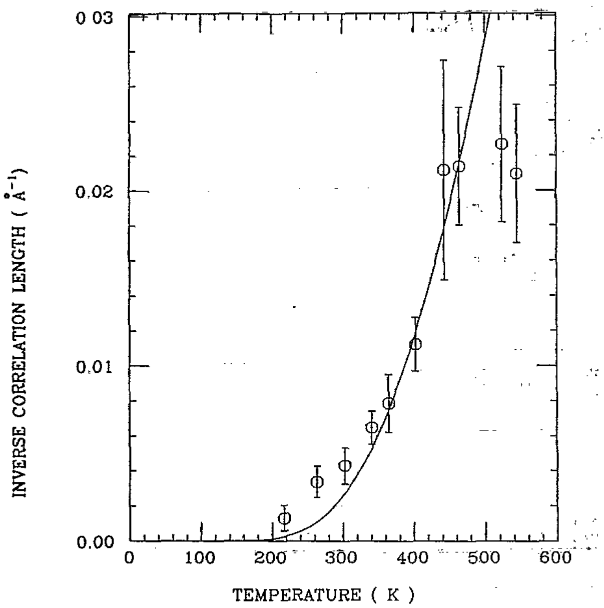


FIG. 3. The solid line corresponds to an exponential fit to our results for both the nonlinear $\sigma$ model and the spin-$\frac{1}{2}$ AF Heisenberg model, taking for the AF coupling the value $J=1270$ K. The open circles with error bars are neutron-scattering data taken on the insulator $La_2CuO_4$.

gin of the discrepancy may be that their improved algorithm searches the phase space more efficiently. We believe that the discrepancy could also be due to finite-size effects which may affect the two calculations differently because the correlation functions have been calculated in different ways. Notice that the correlation length (Fig. 6 of Ref. 15) at, for example, temperature $T/J=0.5$ systematically increases by increasing the size of their lattice. In our calculation finite-size effects appear at larger correlation lengths (somewhat lower temperature). Hence, our results (dashed line in their Fig. 6) may approximate the infinite system better. Nevertheless, using the values for $A_H=0.32$ and $B_H \simeq 1$ reported by GJN, we obtain $\hbar c \simeq 0.93 J a_H$, which is somewhat lower than our value. If, on the other hand, we use the most recent form of CHN,[11] who find $A_H=0.467$ and $B_H=0.94$, we find $\hbar c \simeq 1.27 J a_H$, which is closer to Oguchi's result.

In Fig. 3 we plot the inverse correlation length versus $T$ as observed by neutron-scattering experiments.[2] The solid curve is the exponential given by Eq. (12) which fits both the nonlinear $\sigma$ model and the AF Heisenberg model. In the plot we used $a_H=3.8$ Å, the Cu-Cu distance, and $J=1270$ K, which is close to the value reported by Raman scattering experiments.[10] Our curve disagrees with the data very close to the 3D Néel critical temperature $T_N \sim 200$ K. Smaller values of $J$ will bring our results closer to the data in that region but further away from the data at higher $T$.

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