Crossover and Order-Disorder Transition of Two-Dimensional Quantum Antiferromagnets at Low Temperatures

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We study the low-temperature behavior of quantum antiferromagnets in two space dimensions. Our model is the quantum nonlinear σ model (NLσM), which is the long-wavelength limit of the two-dimensional quantum Heisenberg model. Introducing fermion fields in NLσM, we propose a model of doped antiferromagnets. We show that renormalization-group theory predicts an order-disorder transition at finite hole concentration δ_c. Very small doping changes the temperature dependence of the correlation length ξ from exponential to power law, $\xi \propto 1/T$, for hole concentration $\delta < \delta_c$. We also discuss a crossover between classical and quantum regions with varying coupling constant g.

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Since the discovery of high-temperature superconductors [1], there has been a considerable amount of work done to understand the properties of the oxide superconductors. The undoped oxide compounds exhibit a rich structure of two-dimensional antiferromagnetic correlations over a wide temperature range [2–4]. A simple description of the system is provided by the quantum Heisenberg model. It has been established that the low-temperature, long-wavelength behavior of a two-dimensional quantum antiferromagnet can be described by a quantum nonlinear σ model in two space and one time dimensions [5–7]. The effective action of the nonlinear σ model (NLσM) is defined in the form

$$S=\frac{1}{2g}\int_0^\beta dx_0\int d^2x(\partial_\mu\varphi)^2\,, \tag{1}$$

where φ is an n-component field with the constraint $\varphi^2=1$, g is the dimensionless coupling constant, and β is the dimensionless thickness in the time direction, defined by $\beta=g/t$ where $t=k_BT/JS^2$ [7]. It is also considered that a small number of holes introduced by doping are responsible for the disappearance of long-range antiferromagnetic correlations. The doped materials may be well modeled by the spin systems with frustration, such as the t-J model [8,9] or the Kondo lattice (spin fermion) model [10,11].

This paper consists of two parts. First, we discuss a crossover between classical and quantum regions by evaluating the correlation function. We show that its exponent depends on the magnitude of g. In the second part we propose a model of holes in the quantum spin systems and investigate its effects on the magnetic correlations based on renormalization-group theory. We show that very small hole doping changes the temperature dependence of the correlation length ξ from exponential to power law: $\xi \sim (1/\delta T)\ln(1/T)$.

Now we try to make a $1/n$ expansion. Let us consider a functional integral of the form

$$Z=\int d\lambda(x_0,x)\int d\varphi(x_0,x)\exp\left[-\frac{1}{2g}\int_0^\beta dx_0\int d^2x[(\partial_\mu\varphi)^2+\lambda(\varphi^2-1)]\right]. \tag{2}$$

Here the field $\lambda(x_0,x)$ is introduced to ensure the constraint $\varphi^2=1$. The integral over φ can be performed in a standard fashion. If we take n to be large, we could expect that the saddle-point approximation works well assuming that $\lambda=m^2$ is constant. Then we obtain $m=(2/\beta)\sinh^{-1}[\exp(-2\pi\beta/ng)\sinh(2\pi\beta/ng_c)]$, where g_c is the critical coupling constant given by $g_c=(4\pi/\Lambda)/n$ with a high-energy cutoff $\Lambda=1/a$. The long-distance behavior of the correlation function $\langle\varphi(0)\varphi(R)\rangle$ is well known and its properties can be described by the classical model when the model has long-range order at $T=0$ [7]. Here we focus on the short-distance behavior for $R \ll 1/m$; in this region quantum corrections are responsible for the correlation functions. We show that the exponent η depends on the coupling constant g and there is a crossover between the quantum region for $t \ll g \leq g_c$ and the classical region for $g \ll t$. In the leading-order $1/n$ theory, the short-distance correlation is approximately given by

$$\langle\varphi(0)\varphi(R)\rangle \approx \frac{ng}{4\pi}\frac{2}{\beta}\ln\left|\frac{\sinh(\beta/2R)}{\sinh(\beta m/2)}\right|. \tag{3}$$

At low temperatures $t \ll 1$, in the classical region we obtain

$$\langle\varphi(0)\varphi(R)\rangle \approx 1-\frac{nt}{2\pi}\ln\left(\frac{R}{a}\right)+O\left[\ln\left(\frac{R}{a}\right)\right]^2$$

$$\approx\left(\frac{a}{R}\right)^{nt/2\pi}, \tag{4a}$$

and, in contrast, in the quantum region

$$\langle\varphi(0)\varphi(R)\rangle \approx 1-\frac{ng}{4\pi}\left(\frac{1}{a}-\frac{1}{R}\right)$$
$$\approx 1-\frac{g}{g_c}\ln\left(\frac{R}{a}\right)\approx\left(\frac{a}{R}\right)^{g/g_c}. \qquad (4b)$$

Thus the exponent depends upon the magnitude of g and its expression is given by

$$\eta=-\frac{nt}{2\pi}\frac{d\ln[\sinh(\beta/2R)]}{d\ln R}\bigg|_{R=a}=\frac{ng}{4\pi a}\coth\left(\frac{g}{2ta}\right). \qquad (5)$$

It is remarkable that the crossover function is simply given by $\coth(g/2t)$ which, as shown later, also appears in the β functions of renormalization-group theory to connect classical and quantum regions smoothly. As we can see from Eqs. (4a) and (4b), we have $\langle\varphi(0)\varphi(a)\rangle=1$ because the constraint $\varphi^2=1$ is satisfied for $R\le a$. Thus we have found the crossover between quantum and classical regions as the coupling constant g is reduced. To summarize our results, we show the phase diagram in Fig. 1.

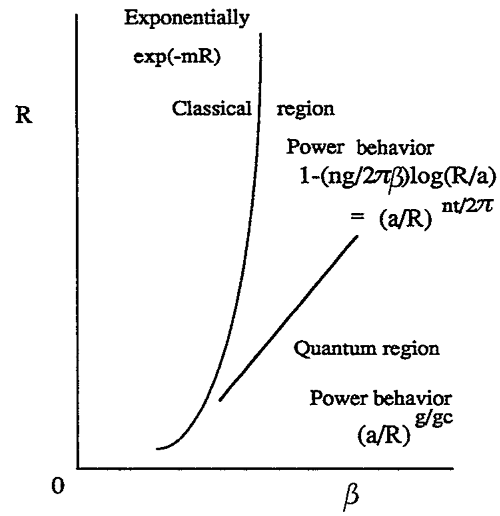

FIG. 1. While the long-distance correlation decays exponentially as e^{-mR}, the short-distance behavior for $R\ll 1/m$ is given by $\langle\varphi(0)\varphi(R)\rangle\approx 1-(ng/2\pi\beta)\ln(R/a)\approx(a/R)^{nt/2\pi}$ in the classical region and $\langle\varphi(0)\varphi(R)\rangle\approx(a/R)^{g/g_c}$ in the quantum region, respectively.

The properties of a doped quantum antiferromagnet are the subject of the remainder of this paper. Our effective action is the following [12]:

$$S=\frac{1}{2g}\int_0^\beta dx_0\int d^2x(\partial_\mu\varphi)^2+\int_0^\beta dx_0\int d^2x\sum_\sigma\psi_\sigma^\dagger\left(\frac{\partial}{\partial x_0}+\varepsilon(\partial)-\mu\right)\psi_\sigma, \qquad (6)$$

with the constraint $\varphi^2+\sum_\sigma\psi_\sigma^\dagger\psi_\sigma=1$. If no hole is present, we obtain $\varphi^2=1$, whereas we have $\varphi(x)^2=0$ if a hole exists at x, which represents a frustration of neighboring spins caused by doped holes. Thus we expect that our model is adequate to discuss the role of holes doped in the ordered spin systems. We assume that the hole concentration $\delta=\langle\sum_\sigma\psi_\sigma^\dagger\psi_\sigma\rangle$ is small, and expand physical quantities in powers of δ. For simplicity, we set the dispersion relation as $\varepsilon_{\mathbf{q}}=|\mathbf{q}|$. First, we evaluate the correlation function in the range where $m<\delta/n\beta$ and $\delta R/n\beta<1$: $\langle\varphi(0)\varphi(R)\rangle\approx(ng/2\pi\beta)\ln(1/\delta TR)$. This formula should be compared with Eq. (3) in the classical regime for $\beta<R<1/m$: $\langle\varphi(0)\varphi(R)\rangle\approx(ng/2\pi\beta)\ln(1/mR)$. Then it is evident that the excitation gap m is replaced by δT if $m<\delta T$ and consequently the correlation length ξ is given by $\xi\propto 1/\delta T$. Hence in the doped case, ξ drastically changes its behavior and obeys a power law in place of an exponential one.

It is physically expected that above the critical concentration δ_c, there is a transition to the disordered state at $T=0$. In order to discuss this transition, it is convenient to use the renormalization-group theory. Following standard conventions, we denote the φ field by $\varphi=(\sigma,\pi)$ where we take σ along the direction of mean magnetization with the assumption that fluctuations about this direction are small. We follow the renormalization procedure of Wilson and Kogut [13], and remove π's with $e^{-\lambda}<q<1$ for infinitesimal λ. Rescaling momenta by e^λ and the field π by ζ, we obtain an action of the original form [7,14,15]. For the undoped quantum spin systems, β functions are already known up to lower-loop orders for $d=2$ [7,16,17],

$$-\beta_g(\lambda)=\frac{dg}{d\lambda}=-g+\frac{n-2}{4\pi}g^2\coth\left(\frac{g}{2t}\right)+\frac{n-2}{(2\pi)^2}g^3\left[\frac{1}{2}\coth\left(\frac{g}{2t}\right)\right]^2, \qquad (7a)$$

$$-\beta_t(\lambda)=\frac{dt}{d\lambda}=\frac{n-2}{4\pi}gt\coth\left(\frac{g}{2t}\right)+\frac{n-2}{(2\pi)^2}g^2t\left[\frac{1}{2}\coth\left(\frac{g}{2t}\right)\right]^2. \qquad (7b)$$

The last terms in Eqs. 7(a) and 7(b) are two-loop contributions. In two limiting cases $g\gg t$ and $g\ll t$, the above β functions are reduced, respectively, to that of the quantum antiferromagnetic Heisenberg model and that of the classical NLσM in two space dimensions up to two-loop order [17]. This crossover is simply described by $\coth(g/2t)$ as η in Eq.

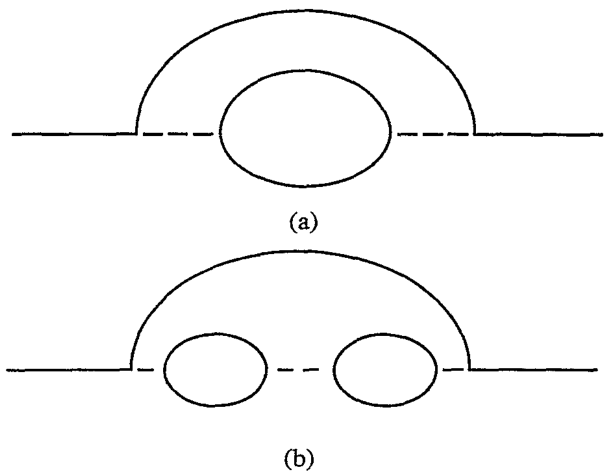

FIG. 2. Feynman diagrams which contribute to the β functions. Closed loops in (a) and (b) are fermion loops and other solid lines indicate π-field propagators.

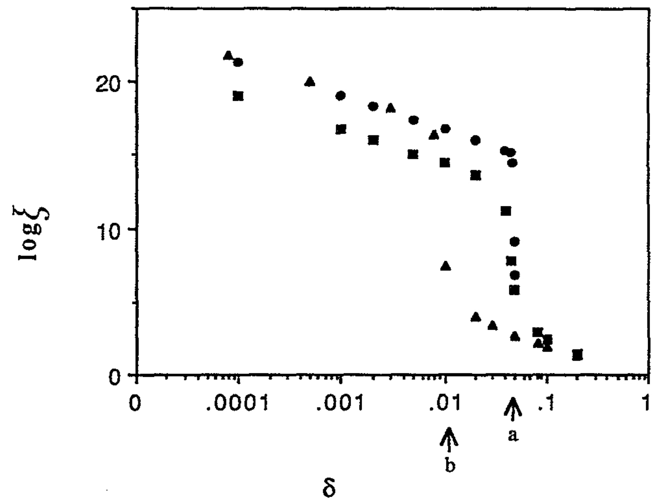

FIG. 3. $\ln\xi$ vs δ. Parameters are as follows: $\beta=10^4$ (circles) and 10^3 (squares) for $g/g_c=0.95$, and $\beta=10^4$ for $g/g_c=0.99$ (triangles). Arrows a and b indicate the position of δ_c: a for $g/g_c=0.95$ and b for $g/g_c=0.99$.

(5) is. Integrating the β functions until the renormalized correlation length $e^{-\lambda}\xi$ is equal to the lattice constant, we can obtain the correlation length ξ. In the case without hole doping, ξ ultimately diverges exponentially as $T\rightarrow 0$ [7,18–21],

$$\xi=(JS/T)^{1-1/(n-2)}\exp[(2\pi JS^2/T)(1/g-1/g_c)]\,.$$

An inessential preexponential factor is modified in two-loop-order renormalization and, as easily shown, higher-order terms are negligible at low temperatures [7]. In order to consider holes in the spin systems, we expand the nonlinearities of the square root $\sigma=(1-\pi^2-\sum_\sigma\psi_\sigma^\dagger\psi_\sigma)^{1/2}$ to do a perturbative analysis in g and δ. It is easily shown that $1/g$ is replaced by $(1-\delta)/g$ in the mean-field approximation for the fermion fields, which leads to the critical coupling constant $g_c^{\rm mean}=(1-\delta)g_c$ where g_c is that for the undoped case. For one-loop order $g_c=4\pi/(n-2)$ and for two-loop order $g_c=[4\pi/(n-2)]\times(\sqrt{5}-1)/2$. A factor $1-\delta$ shows a reduction of g_c due to doped fermions in the mean-field treatment. For $g<g_c^{\rm mean}$, there is the long-range Néel order at $T=0$. Then we consider nontrivial contributions of fermions in one-loop order, as shown in Fig. 2(a):

$$-\beta_g(\lambda)=-g+\frac{n-2}{4\pi}\frac{1}{1-\delta}g^2\coth\left(\frac{g}{2t}\right)+\frac{1}{8\pi}g\delta\coth\left(\frac{g}{2t}\right)+O(\delta^2)\,,\qquad(8a)$$

$$-\beta_t(\lambda)=\frac{n-2}{4\pi}\frac{1}{1-\delta}gt\coth\left(\frac{g}{2t}\right)+\frac{1}{8\pi}t\delta\coth\left(\frac{g}{2t}\right)+O(\delta^2)\,.\qquad(8b)$$

The diagram, which is of the order of δ^2, is shown in Fig. 2(b).

Now let us discuss the correlation length ξ in the doped case for $g<g_c$. We present $\ln\xi$ vs δ for $g/g_c=0.95$ and 0.99 in Fig. 3. An important comment is that although the two-loop term in Eq. 7(b) reduces g_c, it does not change the behavior of ξ as a function of δ for fixed g/g_c, as verified numerically and also analytically [17]. It is clear from this figure that small doping greatly reduces the correlation length ξ. Obviously there is a critical value δ_c of δ. At $\delta=\delta_c$, the correlation length ξ decreases rapidly and changes its behavior as a function of temperature. In fact, in the region $0<\delta<\delta_c$, ξ shows a power law $\xi\propto 1/T$ as shown in Fig. 4, similar to the one-

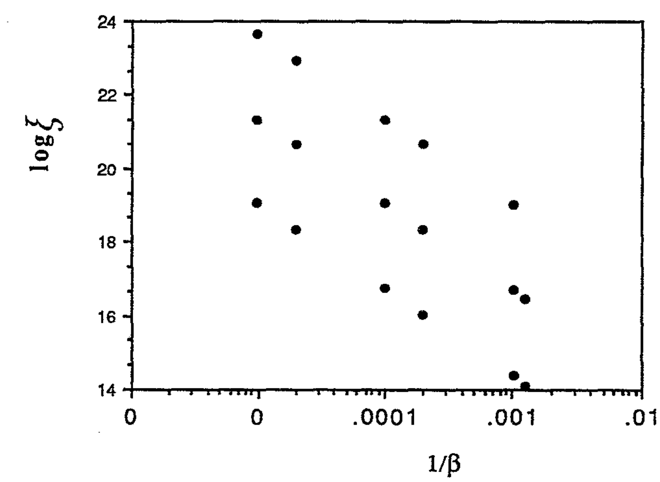

FIG. 4. $\ln\xi$ vs $\log_{10}(1/\beta)$ for $\delta<\delta_c$. From the top, $\delta=10^{-4}$, 10^{-3}, and 10^{-2}.

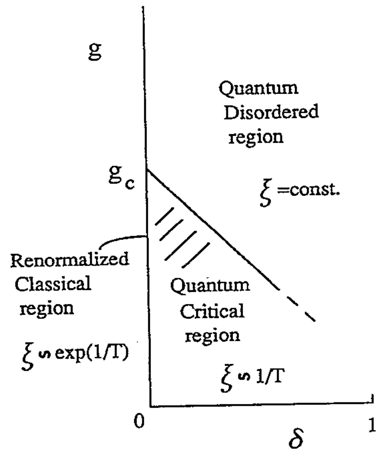

FIG. 5. Crossover diagram in the g-δ plane.

dimensional quantum spin systems, while in the classical region $\delta=0$, ξ diverges exponentially. This result is consistent with that of the $1/n$ expansion. An analysis on Eqs. (8a) and (8b) easily leads to the following expression: $\xi=(\beta/2)\{1+(8\pi/\delta)\ln[2\pi\beta(1/g-1/g_c)]\}$. The logarithmic correction $\ln(1/t)$ gives a minor correction at low temperatures. In the quantum critical region for $0<\delta<\delta_c$, $t(\lambda)$ grows faster than $g(\lambda)$ so that we choose λ_* such that $t(\lambda_*)=1$. We obtain ξ by a formula $\xi=ae^{\lambda_*}$ where a is the lattice constant. In the quantum disordered region for $\delta>\delta_c$, the solution of Eqs. 8(a) and 8(b) shows that $g(\lambda)$ grows faster than $t(\lambda)$ and ξ becomes independent of temperature as $T\to 0$. Then we can say that at the critical point $\delta=\delta_c$ there is a transition to the disordered state at $T=0$. The value of δ_c is linearly dependent on g/g_c if $1-g/g_c$ is small.

In summary we show the phase diagram presented in Fig. 5 where there are three distinct regions characterized by the behavior of ξ as a function of temperature: (i) $\delta=0$, the renormalized classical region; (ii) $0<\delta<\delta_c$, the quantum critical region; and (iii) $\delta_c<\delta$, the quantum disordered region. In the classical region ξ diverges ultimately exponentially as $T\to 0$ and in the quantum critical region ξ obeys the power law. Finally, in the quantum disordered region ξ is independent of T. Thus we have shown the order-disorder transition induced by holes doped in a two-dimensional quantum antiferromagnet.

[1] C. Bednorz and J. A. Muller, Z. Phys. B **64**, 189 (1986).
[2] G. Shirane, Y. Endoh, R. Birgeneau, M. A. Kastner, Y. Hidaka, M. Oda, M. Suzuki, and T. Murakami, Phys. Rev. Lett. **59**, 1613 (1987).
[3] K. B. Lyons, P. A. Fleury, L. F. Schneemeyer, and J. V. Waszczak, Phys. Rev. Lett. **60**, 732 (1988).
[4] G. Aeppli and D. J. Buttrey, Phys. Rev. Lett. **61**, 203 (1988).
[5] F. D. M. Haldane, Phys. Rev. Lett. **50**, 1153 (1983).
[6] I. Affleck, Nucl. Phys. **B257**, 397 (1985).
[7] S. Chakravarty, B. I. Halperin, and D. R. Nelson, Phys. Rev. B **39**, 2344 (1989).
[8] A. B. Harris and R. V. Lange, Phys. Rev. **157**, 295 (1967).
[9] F. C. Zhang and T. M. Rice, Phys. Rev. B **37**, 3759 (1988).
[10] P. Prelovsek, Phys. Lett. A **126**, 287 (1988).
[11] M. Ogata and H. Shiba, J. Phys. Soc. Jpn. **57**, 3074 (1988).
[12] T. Yanagisawa, J. Phys. Soc. Jpn. (to be published).
[13] K. G. Wilson and J. Kogut, Phys. Rep. **12**, 75 (1974).
[14] A. M. Polyakov, Phys. Lett. **59B**, 79 (1975).
[15] D. R. Nelson and R. A. Pelcovits, Phys. Rev. B **16**, 2191 (1977).
[16] E. Brezin and J. Zinn-Justin, Phys. Rev. B **14**, 3110 (1976).
[17] T. Yanagisawa (to be published).
[18] E. Manousakis and R. Salvador, Phys. Rev. Lett. **62**, 1310 (1989).
[19] H.-Q. Ding and M. S. Makivic, Phys. Rev. Lett. **64**, 1449 (1990).
[20] G. Gomez-Santos, J. D. Joannopulos, and J. W. Negel, Phys. Rev. B **39**, 4435 (1989).
[21] E. Manousakis, Rev. Mod. Phys. **63**, 1 (1991).