# Quantum Phase Transitions in *XY* Spin Models

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The ground state of an *XY* model changes at a critical transverse field, above which there is a gap from the fully polarized ground state to the first excitation. We investigate the phase transition from this "Mott insulator" phase as the transverse field approaches its critical value. We calculate exactly some Green's functions and critical exponents for $d$-dimensional ferromagnetic lattices and for the Sherrington-Kirkpatrick spin-glass model. Finite-dimensional spin glasses are also discussed.

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The past few years have seen a major increase in activity in the field of strongly interacting systems. Parallel to the intensive study of fermionic problems, there is an increasing appreciation of the relevance of bosonic issues. In particular, problems in the presence of disorder have attracted much attention recently. Since the spin-1/2 *XY* model is equivalent to the lattice gas of hard-core bosons, this model has been used to describe experimental systems whose essence is adequately captured by bosonic physics: $^4$He in disordered media [1] or high-$T_c$ superconductors [2] in which the Cooper pairs may act like bosons. Very recent developments make it plausible that in high-$T_c$ materials the symmetry of the order parameter is of $d$ type [3]. When granular $d$-wave superconductors are mapped on the equivalent spin problem they give rise to random exchange couplings, i.e., a spin-glass problem [4]. The quantum spin-glass model has been studied mainly for infinite-range interactions, i.e., for the Sherrington-Kirkpatrick (SK) model [5–7], though there are some Monte Carlo results in two [8] and three dimensions [9] for Ising spin glasses in a transverse field.

In this paper we investigate the quantum *XY* model for a general spin $S$, with and without disorder, paying special attention to the spin-glass problem. We present some exact results for the Mott insulator (MI) to superfluid (long-range ordered) phase transition, which have been investigated extensively with field theoretical [10], exact diagonalization [11], and Monte Carlo methods [12]. Our model is defined by the Hamiltonian

$$\tilde{H} = -\frac{1}{2}\sum_{i\neq j}^{N} J_{ij}(S_i^x S_j^x + S_i^y S_j^y) - K\sum_{i=1}^{N} S_i^z + KNS, \quad (1)$$

where $\mathbf{S}_i = (S_i^x, S_i^y, S_i^z)$ is the quantum spin operator associated with the local spin $S$ at site $i = 1,\ldots,N$. $J_{ij}(i < j,\ J_{ij} = J_{ji})$ is an element of the exchange-interactions matrix $J$, and $K$ is the strength of the transverse field. As we have shown [13], for $K > K_c$, the ground state of the Hamiltonian (1) is the fully polarized state $|NS\rangle$, where all spins are aligned in the $z$ direction, i.e., the total magnetization $M_z = \sum_i S_i^z$ is $NS$. The critical value $K_c$ depends only on the highest eigenvalue $J_{\max}$ of $J$ and on the spin $K_c = SJ_{\max}$. The constant $KSN$ in the Hamiltonian (1) ensures that the state $|NS\rangle$ has zero energy.

We rescale the Hamiltonian (1) as $H = \tilde{H}/S$ and introduce the operators

$$n_i = S - S_i^z, \qquad a_i^+ = \frac{S_i^-}{\sqrt{2S}}, \qquad a_i = \frac{S_i^+}{\sqrt{2S}}, \quad (2)$$

where $S^{\pm} = S^x \pm iS^y$. The operator $n_i$ gives the difference to the fully polarized state at site $i$ (number of holes) and the operator $a_i^+(a_i)$ creates (annihilates) a hole at site $i$. From these definitions one obtains the commutation relation $[a_i, a_j^+] = \delta_{ij}(1 - n_i/S)$ and the rescaled Hamiltonian is

$$H = -\sum_{i,j} J_{ij} a_i^+ a_j + \mu\sum_i n_i, \qquad \mu = \frac{K}{S}. \quad (3)$$

Since the operator $\mathcal{N} = \sum_i n_i$ commutes with $H$ in Eq. (3), we can characterize the eigenstates of $H$ by a given $\mathcal{N}$: for $\mu > \mu_c = J_{\max}$ the ground state is $|NS\rangle$, for which $\mathcal{N} = 0$.

In the $\mathcal{N} = 1$ subspace the eigenstates of $H$ can be found by diagonalizing $J$: $J\mathbf{v}^k = J_k\mathbf{v}^k$, where $\mathbf{v}^k = (v_1^k,\ldots,v_i^k,\ldots,v_N^k)$ is a normalized eigenvector. With the help of the new operators

$$b_k = \sum_i v_i^k a_i, \qquad b_k^+ = \sum_i (v_i^k)^* a_i^+ \quad (k = 1,\ldots,N), \quad (4)$$

for which the commutation relations are

$$[b_k, b_q^+] = \delta_{kq} - \frac{1}{S}\sum_i v_i^k (v_i^q)^* n_i, \quad (5)$$

one obtains

$$H = -\sum_k J_k b_k^+ b_k + \mu\sum_i n_i. \quad (6)$$

From Eqs. (5) and (6) can be shown that the state $|k\rangle \equiv b_k^+|NS\rangle$, $k = 1,\ldots,N$, is an eigenstate of the Hamiltonian (6),

$$H|k\rangle = (\mu - J_k)|k\rangle. \quad (7)$$

This implies that for $\mu > \mu_c$ there is a gap $\mu - \mu_c$ between the $\mathcal{N} = 0$ and $\mathcal{N} = 1$ subspaces. In Ref. [13] we have proved rigorously that this also holds for $\mathcal{N} >$

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1: denoting by $E_{\mathcal{N}}$ the energy of a state in the subspace $\mathcal{N}$, we have

$$E_{\mathcal{N}} \geq (\mu - \mu_c)\mathcal{N} . \tag{8}$$

This means that for $\mu > \mu_c$ we know the ground state and the first excitations exactly, which enables us to calculate the imaginary-time Green's function

$$g(\mathbf{r}_i, \mathbf{r}_j; \tau, \tau') = \langle T_\tau a_i(\tau) a_j^+(\tau') \rangle , \tag{9}$$

where $A(\tau) = \exp(\tau H) A \exp(-\tau H)$ and $T_\tau$ orders the operators in decreasing time arguments. The angular brackets refer to the ground state expectation value. Since there is no "hole" excitation in the ground state $|NS\rangle$, $g(\mathbf{r}_i, \mathbf{r}_j; \tau, \tau') = 0$ for $\tau < \tau'$. On the other hand, $g$ depends only on the difference $\tau - \tau'$, so we can set $\tau' \equiv 0$. Inverting Eq. (4) and using Eq. (7) gives

$$g(\mathbf{r}_i, \mathbf{r}_j; \tau) = \begin{cases} \sum_k v_i^k (v_j^k)^* e^{-\tau(\mu - J_k)} & \text{if } \tau \geq 0, \\ 0 & \text{otherwise.} \end{cases} \tag{10}$$

*(1) Ferromagnetic lattices.*—Equation (10) is valid for any $J$, though we know the eigenvectors explicitly only for periodic systems. For a $d$-dimensional ferromagnetic cubic lattice of size $N = L^d$ the eigenvectors of $J$ can be enumerated by introducing the wave vector $\mathbf{k}$: $v_j^{\mathbf{k}} = L^{-d/2} \exp(i\mathbf{k} \cdot \mathbf{r}_j)$, $j = 1, \ldots, L^d$, $k_\alpha = n_\alpha 2\pi/L$ with $\alpha = 1, \ldots, d$, and $n_\alpha = -L/2, \ldots, L/2$ for unit lattice spacing. The eigenvalues of $J$ are $J_{\mathbf{k}} = 2J \sum_\alpha \cos k_\alpha$, where $J$ is the strength of the nearest-neighbor interactions. Since the lattice is periodic, $g(\mathbf{r}_i, \mathbf{r}_j; \tau)$ depends only on the distance $\mathbf{r} = \mathbf{r}_i - \mathbf{r}_j$:

$$g(\mathbf{r}; \tau) = e^{-\tau\mu} L^{-d} \sum_{\mathbf{k}} \exp\left( i\mathbf{k} \cdot \mathbf{r} + 2J\tau \sum_\alpha \cos k_\alpha \right). \tag{11}$$

In the limit $L \to \infty$ the sum $L^{-d} \sum_{\mathbf{k}}$ in Eq. (11) can be replaced by an integral, giving

$$g(\mathbf{r}; \tau) = e^{-\tau\mu} \prod_\alpha \mathbf{I}_{r_\alpha}(2J\tau) , \tag{12}$$

where $\mathbf{I}_n(x)$ is the modified Bessel function of integer order. The Fourier transform $G(\mathbf{k}, \omega)$ of $g(\mathbf{r}; \tau)$ is given by

$$G^{-1}(\mathbf{k}; \omega) = i\omega + \mu - 2J \sum_{\alpha=1}^{d} \cos k_\alpha . \tag{13}$$

Equations (12) and (13) give the exact Green's function for the ferromagnetic cubic lattice in the MI phase, i.e., for $\mu > \mu_c = J_{\max} = 2Jd$. Approaching the transition from above $G(\mathbf{k}; \omega)$ [Eq. (13)] can be approximated for $k \ll 1$ as

$$G^{-1}(\mathbf{k}; \omega) \longrightarrow i\omega + Jk^2 + \delta, \quad \text{with} \quad \delta = \mu - \mu_c . \tag{14}$$

For $\omega = 0$ there is a diverging correlation length $\xi \propto \delta^{-\nu}$ in the space direction. From Eq. (14) it is seen that $\nu = 1/2$. Right at the transition point $G(\mathbf{k}; \omega) \propto k^{-2}$, which gives $\eta = 0$ for the power-law decay of the space correlations. Since the gap disappears linearly with $\delta$ [Eq. (8)], the correlation length in the imaginary-time direction is $\xi_\tau \propto \delta^{-1}$, which gives a dynamical exponent $z = 2$ through the relation $\xi_\tau \propto \xi^z$.

The correlations in the imaginary-time direction can be studied directly from Eq. (12). For any finite $r$ and $\tau \to \infty$ we have

$$g(\mathbf{r}; \tau) \longrightarrow \frac{1}{(4\pi J)^{d/2}} \frac{e^{-\tau\delta}}{\tau^{d/2}} , \tag{15}$$

showing that the relation $z\nu = 1$ is satisfied in any dimension $d$ and the power-law decay at the transition point ($\delta = 0$) fulfills the scaling relation $(d + z - 2 + \eta)/z = d/2$ [10]. In $d = 1$ the space correlations can be calculated explicitly, giving

$$g(\mathbf{r}) = \int_0^\infty g(\mathbf{r}; \tau)\, d\tau = \frac{1}{\sqrt{\mu^2 - \mu_c^2}} \exp(-\mathbf{r}/\xi) , \tag{16}$$

$$\xi^{-1} = \ln \frac{\mu + \sqrt{\mu^2 - \mu_c^2}}{\mu_c} . \tag{17}$$

In the limit $\delta \to 0$, $g(\mathbf{r}) \propto r\tilde{g}(r/\xi)$, with the scaling function $\tilde{g}(x) = \exp(-x)/x$ and $\xi \propto \delta^{-1/2}$, in accordance with the general $d$-dimensional result $\nu = 1/2$, $\eta = 0$, and $z = 2$ obtained from Eq. (14).

*(2) Disordered systems.*—In the disordered case it is difficult to study the space correlations because this requires knowledge of the eigenvectors of $J$. Nevertheless, to see the imaginary-time behavior of $g(\mathbf{r}_i, \mathbf{r}_j; \tau)$ we can calculate from Eq. (10) the average on-site correlation

$$g(\tau) = \frac{1}{N} \sum_i g(\mathbf{r}_i, \mathbf{r}_i; \tau) = \int d\lambda\, \varrho(\lambda) e^{-\tau(\mu - \lambda)}, \tag{18}$$

where $\varrho(\lambda) = N^{-1} \sum_k \delta(\lambda - J_k)$ is the density of states of $J$, and $\delta(x)$ is the Dirac delta function. Equation (18) shows that the imaginary-time correlations can be obtained using the spectrum of $J$ in the MI phase, i.e., for $\mu > \mu_c$.

The most celebrated example of a disordered system whose spectrum is known in the limit $N \to \infty$ is that in which, for all pairs $(i, j)$, $J_{ij}$ are random numbers governed by independent symmetric Gaussian distributions with mean zero and variance $1/\sqrt{N}$. This SK model possesses a semicircular spectrum [14] $\varrho(\lambda) = (2\pi)^{-1}\sqrt{4 - \lambda^2}$ and the transition occurs [7,13] at $\mu_c = 2$. Putting this expression into Eq. (18) gives

$$g_{\mathrm{SK}}(\tau) = \frac{e^{-\tau\mu}}{\tau} \mathbf{I}_1(2\tau) \quad \text{for} \quad \mu > \mu_c , \tag{19}$$

where $\mathbf{I}_1(x)$ is the modified Bessel function of first order. Equation (19) is the exact imaginary-time correlation function of the $XY$ SK spin-glass model in the MI phase. Its critical behavior in the limit $\tau \to \infty$ is

$$g_{\mathrm{SK}}(\tau) \simeq \frac{e^{-\tau\delta}}{\tau^{3/2}} . \tag{20}$$

The correlation length in the imaginary-time direction is $\xi_\tau = \delta^{-1}$ and at the phase transition ($\delta = 0$) the correlation function decays as $g_{SK}(\tau) \propto \tau^{-3/2}$. We recall that Miller and Huse [6] obtained $g(\tau) \propto \tau^{-2}$ for the Ising SK spin-glass model.

For the SK model the transition to the spin-glass state occurs when the local susceptibility $\chi_0$ becomes 1. $\chi_0$ can be calculated from the spin correlation function $C_{xx}(\tau) = \langle T_\tau S_x(\tau) S_x(0)\rangle$ by integrating over $\tau$:

$$\chi_0 = \int_{-\infty}^{\infty} C_{xx}(\tau)\, d\tau = \int_0^{\infty} g(\tau)\, d\tau . \tag{21}$$

In the last equality we have used the rescaling relations of Eq. (2) and the fact that $C_{xx}(\tau)$ is an even function of $\tau$. Integration of Eq. (19) gives

$$\chi_0(\mu) = \frac{1}{2}\left(\mu - \sqrt{\mu^2 - 4}\right). \tag{22}$$

As one can see, $\chi_0(\mu_c) = 1$, which confirms our previous conjecture [7] based on finite Trotter-Suzuki calculations and on some physical arguments which say that the spin-glass transition occurs at $\mu_c$.

It is remarkable that the static approximation [5] gives the same $\chi_0$ as Eq. (22) for $T = 0$ [15]. Although we have no explanation for this coincidence, we recall that the static approximation introduces two errors [7]: $\langle S_x(\tau) S_x(0)\rangle$ is supposed to be constant and $\langle S_x(\tau) S_y(0)\rangle$ is completely neglected. These two errors seem to cancel each other out in the expression of $\chi_0$.

Putting the $\chi_0$ of Eq. (22) into the expression for the bulk nonlinear susceptibility $\chi_2^B$ [16], we have

$$\chi_2^B \propto \frac{1}{1 - \chi_0^2} = \frac{1}{\chi_0}\frac{1}{\sqrt{\mu^2 - 4}} . \tag{23}$$

Near the transition, $\mu \to \mu_c$, $\chi_2^B$ diverges as $\delta^{-\gamma}$ with $\gamma = 1/2$. Comparing this result to that obtained for the Ising model [6] we find the same exponent $\gamma = 1/2$, but without the logarithmic correction present in the Ising case.

*(3) Finite-dimensional spin glasses.*—In both the ferromagnetic and the SK spin-glass cases the transition occurs from the MI state to a superfluid phase, i.e., to a long-range ordered phase (for $d = 1$ there is a quasi-long-range order). In these models the eigenvector of the highest eigenvalue is an extended state, which means that each element of this vector is of the order of $1/\sqrt{N}$. Thus the last "disturbing" term in the commutation relation of Eq. (5) can be estimated as $\mathcal{O}(\mathcal{N}/N)$, implying that for a small number of excitations $\mathcal{N}$ the $b$ operators behave as independent bosons.

For finite-dimensional disordered matrices $J$ the eigenvectors of the highest eigenvalues are localized [17]. One can characterize this localization by the so-called inverse participation ratio (IPR) $P_k = \sum_i |v_i^k|^4$. An example of the IPR of the eigenvectors is shown in Fig. 1. For two nonoverlapping localized eigenvectors $\mathbf{v}^k$ and $\mathbf{v}^q$ the corresponding operators $b_k$ and $b_q$ [Eq. (4)] commute: the last term in Eq. (5) can be neglected. On the other hand,

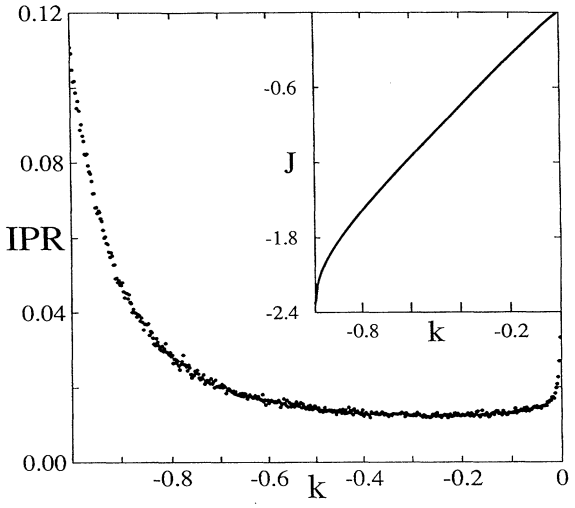


FIG. 1. Inverse participation ratio (IPR) of a $30 \times 30$ square lattice averaged over $10^3$ samples. The nearest-neighbor independent random exchange interactions $J_{ij}$ are uniformly distributed on $[-1, 1]$. Eigenstates of the interaction matrix $J$ are labeled by $k \in [-1, 1]$, $k = -1$ corresponding to the ground state of $J$. The inset shows the averaged spectrum of $J$. Since the IPR is symmetric and the spectrum of $J$ is antisymmetric with respect to $k = 0$ (see Ref. [18]) only their left-half parts are plotted.

for the commutation of $b_k$ and $b_k^+$, this disturbing term will be of the order of 1.

To quantify these ideas, let us estimate the energy of a state containing two excitations $|kq\rangle = b_k^+ b_q^+ |NS\rangle$:

$$H|kq\rangle = [-(J_k + J_q) + 2\mu]|kq\rangle + \frac{1}{S}\sum_{pr} c_{kqpr} J_p |pr\rangle , \tag{24}$$

with $c_{kqpr} = \sum_i (v_i^k)^* (v_i^q)^* v_i^p v_i^r$. If $\mathbf{v}^k$ and $\mathbf{v}^q$ are two different localized states, the biggest contribution in the last term of Eq. (24) comes from $Q_{kq} = c_{kqkq} = \sum_i |v_i^k|^2 |v_i^q|^2$, which is nothing but the overlap of the states $\mathbf{v}^k$ and $\mathbf{v}^q$. If $\mathbf{v}^k$ and $\mathbf{v}^q$ are from the low-lying strongly localized states, one can suppose the corresponding $Q_{kq}$ to be small.

On the other hand, if $k = q$, the biggest contribution in the last term of Eq. (24) comes from $c_{kkkk} = P_k$, which is nothing but the IPR of the $k$th state. Since the IPR of the low-lying localized states is finite, this term gives a finite on-site repulsion. This means that as far as the overlap of the lowest-lying states is small, the corresponding excitations behave like bosons with strong on-site repulsion on a weakly coupled lattice, where the site energies are given by the one-particle energies $J_k - \mu$. The repulsive interaction between the "bosons" insures that slightly below $\mu_c$ only the lowest-lying states be occupied by a small number of bosons.

Though the nature of the coupling between the one-particle states is certainly more complicated than the simple "hopping" of bosons, these details can be irrelevant if the coupling is small enough, i.e., for small bosons

densities. In this case one expects a behavior similar to that of a Bose glass [10]: the imaginary-time correlations decay as $\tau^{-1}$, giving a diverging susceptibility. When $\mu$ is lowered further, and the occupied states more and more overlap a transition from this localized phase the spin-glass phase happens. The study of this transition is beyond the scope of this Letter.

In conclusion, we have studied the phase transitions from the Mott insulating phase for the $XY$ model in a transverse field. The critical exponents $\nu = 1/2$, $z = 2$, and $\eta = 0$ have been obtained for ferromagnetic lattices. We have calculated the exact imaginary-time Green's function of the SK spin-glass model which gives a $\tau^{-3/2}$ decay at the critical point and the nonlinear susceptibility diverges as $(\mu - \mu_c)^{-1/2}$. In the SK spin glass the transition from the MI phase passes directly to the spin-glass state, unlike finite-dimensional spin glasses where there is a localized phase between the MI and the spin-glass phases.

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