Absence of a percolation threshold in a quantum diluted Ising model

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A quantum bond-diluted Ising model is introduced. The model is reducible to its classical corresponding pure Ising model through the standard iteration-decoration transformation. The model considers a finite probability amplitude t for the bond hopping to and from an infinite bond reservoir. The exact phase diagram of the model on a square lattice is obtained and displays no percolation threshold for any finite t. Possible relevance of the present result for systems with hole or electron doping is discussed.

I. INTRODUCTION

The study of models with annealed disorder represents an important tool in dealing with randomly frustrated and diluted systems. Because the thermal and configurational averages are performed by using a common Gibbs factor, the annealed problem is usually easier to treat analytically than the problem of quenched disorder.[1] Although most of the real disordered systems have quenched disorder distribution, the interest in the study of annealed models has increased in the last few years. Annealed bond-disordered models have been used in the investigation of the magnetic properties of the CuO_2 layers present in the doped cuprate superconductors.[2–4] In these systems, hole or electron doping produces frustration effects.[5] Frustration- and fluctuation-induced correlations between the mobile charge carriers have been suggested as possible channels for the effective mechanism of Cooper pairing in these materials.[4–6]

In the annealed models, the equilibrium disorder distribution is constrained by the condition of minimizing the Helmholtz free energy. Due to this constraint, these models are not random at all, in the sense that there are correlations in the disorder distribution, and hence, one must be careful when comparing systems with annealed and quenched disorder. For example, in systems with site dilution, instead of the percolation picture displayed by quenched systems, these correlations lead to a phase-separation transition where the system splits up in site-rich and site-poor phases.[7] On the other hand, for annealed bond-diluted models the correlations in the bond distribution are not strong enough to promote a phase-separation instability, and the phase diagrams of annealed and quenched bond-diluted models are usually quite similar.

In general, the models of annealed dilution follow the original Syozi grand-canonical approach for diluted magnets.[8] The system is supposed to be in contact with a reservoir of particles that can be adsorbed in the intersite bonds and activate a coupling constant between spins located at the vertex of the lattice. The chemical potential μ per activated bond is used as a hidden variable in order to control the mean number of activated bonds. The annealed bond-diluted problem is closely related to the decoration problem and it is exactly solvable once the solution of the corresponding pure model is known.[8,9] A general feature of these models is that there is a critical bond concentration below which no long-range order can be achieved. Also, as a usual feature of phase transition in constrained systems,[10] the universality class of annealed disordered models is distinct from that of its pure counterpart, with its critical exponents becoming renormalized. The percolation concentration p_c is an important characteristic of the system and is known to be dependent on the range of the interactions (but not on their strength), on the geometry and dimensionality of the lattice (but not on the dimensionality of the order parameter), as well as on the nature of the disorder distribution (quenched or annealed).

A quantum version of the bond-diluted problem was introduced by Kirkpatrick and Eggarter[11] as a variation of the tight-binding model of Anderson.[12] In the diluted tight-binding model, the electron is permitted to hop from site to site on a diluted lattice, the hopping being forbidden between sites whose connecting bond has been removed. This model displays a transition between a nonlocalized (metallic) and a localized (insulate) electronic state when the fraction of cut bonds reaches a critical value p_q. The quantum percolation threshold p_q is usually smaller than its classical analog p_c. Scaling arguments indicate that the lower critical dimension for the metal-insulator transition in the Kirkpatrick and Eggarter model is $d_m=2$ (Ref. 13), the electronic states being localized for $d<d_m$ at any finite fraction of cut bonds. The emergence of just a few extended states for $d=2+\epsilon$, in which one may have large electron-phonon interactions, has been used as an indicative of the key role played by quantum percolation in the high transition temperatures attained by the layered copper oxide superconductors.[14]

In this paper a model of bond dilution is introduced where, besides a statistical mixture of the bond configurations, the possibility of quantum mixing is also introduced. More specifically, the states of each bond, namely cut bond $|0>$ and uncut bond $|1>$, are not con-

sidered as steady quantum states but as having a finite probability amplitude t of hopping from one configuration to the other. The model is an extension of the Syozi-like models of diluted magnets, where, instead of considering the interstitial particles as classical objects, it introduces a finite quantum amplitude of probability for the particles to hop from the bond to the reservoir or to be adsorbed back. The generalization to quantum doping particles leads to quite different features displayed in the phase diagram, as, for example, the absence of a critical bond concentration below which long-range magnetic order disappears at $T=0$. For very large t, the phase diagram coincides with the one obtained by the usual mean-field approximation.

II. MODEL AND FORMALISM

One of the major difficulties of dealing with quantum systems with itinerant particles lies in the fact that the eigenstates of the Hamiltonian are linear combinations of the system's configurational particle distribution. This difficulty is even increased when a diluted lattice is introduced. If one were able to construct the Hilbert space of states by a direct product of independent subspaces related to the quantum states of each individual site (bond), this problem would be overcome. Unfortunately, it is not possible to perform such a construction in systems with intersite or interbond hopping, as, for example, in tight-binding models. However, it can be done by assuming that the quantum particles are only allowed to hop to or from an infinite particle reservoir, whose state is considered unchanged during this process, thus avoiding the issues related to the quantum transport. In order to illustrate this approach, an Ising model with such a quantum bond dilution will be considered in the following. The vertex spins σ_i will be considered as localized but the bond distribution is determined by a random adsorption of quantum particles whose presence activates a coupling between the vertex spins. The model can be characterized by the Hamiltonian,

$$\mathcal{H}=\sum_{i,j}\mathcal{H}_{i,j}\ , \tag{1}$$

where $\mathcal{H}_{i,j}$ is a 2×2 matrix Hamiltonian connecting the neighboring sites i and j. Usually its only nonzero element is $\langle 1|\mathcal{H}_{i,j}|1\rangle=-J\sigma_i\sigma_j-\mu$, which means that the Ising spins σ_i and σ_j interact through a coupling parameter J when the bond is uncut. μ is the chemical potential per bond, which is used as a hidden variable in order to control the mean concentration of uncut bonds. In the present model it is also considered that the bond configuration may be quantically mixed, introducing a finite matrix element $\langle 0|\mathcal{H}_{i,j}|1\rangle=\langle 1|\mathcal{H}_{i,j}|0\rangle=t$. This element assures that the bond activation particle has a finite amplitude of probability of hopping to or from an infinite reservoir. The matrix representation of $\mathcal{H}_{i,j}$ is

$$\mathcal{H}_{i,j}=\begin{bmatrix}0 & t\\ t & -J\sigma_i\sigma_j-\mu\end{bmatrix}\ . \tag{2}$$

The partition function of the diluted model can be related to the partition function of the pure model by the decoration transformation that performs a partial trace over all bond configurations:

$$\mathcal{Z}=\mathrm{Tr}_{\sigma_i,\sigma_j}\prod_{i,j}\mathrm{Tr}e^{-\beta\mathcal{H}_{i,j}}=\mathrm{Tr}_{\sigma_i,\sigma_j}A^N\prod_{i,j}e^{\beta J_{\mathrm{eff}}\sigma_i\sigma_j}$$
$$=A^N\mathcal{Z}_0(\beta J_{\mathrm{eff}})\ , \tag{3}$$

where $\mathcal{Z}_0(\beta J_{\mathrm{eff}})$ is the partition function of the pure counterpart model with N connecting bonds and an effective coupling J_{eff}. A and J_{eff} are obtained from the identity,

$$Ae^{\beta J_{\mathrm{eff}}\sigma_i\sigma_j}=\mathrm{Tr}e^{-\beta\mathcal{H}_{i,j}}=e^{-\beta\lambda_+(\sigma_i\sigma_j)}+e^{-\beta\lambda_-(\sigma_i\sigma_j)}\ , \tag{4}$$

$\lambda_\pm$ being the eigenvalues of $\mathcal{H}_{i,j}$,

$$\lambda_\pm(\sigma_i\sigma_j)=\frac{-J\sigma_i\sigma_j-\mu}{2}\pm\frac{1}{2}\sqrt{(J\sigma_i\sigma_j+\mu)^2+4t^2}\ . \tag{5}$$

Equation (5) is satisfied for both $\sigma_i\sigma_j=\pm 1$ when

$$A^2=4e^{\beta\mu}\cosh\left[\frac{\beta}{2}\sqrt{(J+\mu)^2+4t^2}\right]\cosh\left[\frac{\beta}{2}\sqrt{(J-\mu)^2+4t^2}\right]\ , \tag{6}$$

$$e^{J_{\mathrm{eff}}}=e^{J}\cosh\left[\frac{\beta}{2}\sqrt{(J+\mu)^2+4t^2}\right]\Big/\cosh\left[\frac{\beta}{2}\sqrt{(J-\mu)^2+4t^2}\right]\ . \tag{7}$$

The mean concentration of bonds can be obtained as a function of μ, β, J, and t as

$$p=\frac{1}{N}\frac{\partial\ln\mathcal{Z}}{\partial\beta\mu}=\frac{k_BT}{A}\frac{\partial A}{\partial\mu}+\epsilon(\beta J_{\mathrm{eff}})\frac{\partial J_{\mathrm{eff}}}{\partial\mu}\ , \tag{8}$$

and will be used to eliminate the hidden variable μ. Equations (6)–(8) then permit the computation of the exact partition function, once $\mathcal{Z}_0(\beta J_{\mathrm{eff}})$ and $\epsilon(\beta J_{\mathrm{eff}})$ are known. The particular case of a square lattice will be considered as follows. The exact phase diagram can be obtained by imposing that at the transition $\beta J_{\mathrm{eff}}=\beta J_c=0.441$ and $\epsilon(\beta J_c)=\sqrt{2}/2$. In Fig. 1 the phase diagram is plotted in the $T\times p$ plane for various values of t. For $t=0$, the traditional phase diagram for the Ising model with annealed dilution on a square lattice is recovered. However, for any finite t, a percolation threshold is absent and the ground state is always ordered. For small t/J, a crossover from classical to quantum behavior is obtained at low temperatures, characterized by a long tail in the phase diagram. As $t/J\to\infty$ the phase diagram assumes the form obtained in mean-field approximation. In spite of the absence of a percolation

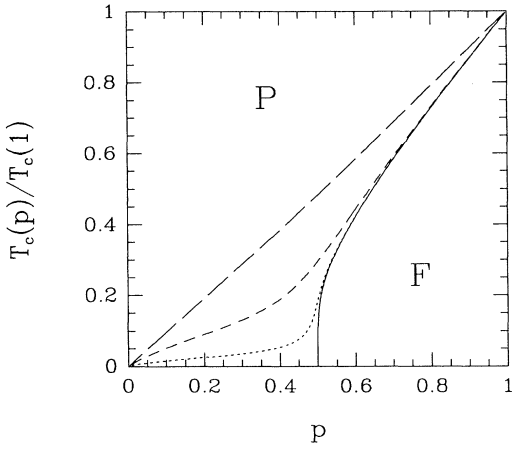

FIG. 1. Phase diagram for the quantum bond-diluted Ising model with finite out-of-plane hopping amplitude in a square lattice for $t/J=0$ (continuous line), $t/J=0.1$ (points), $t/J=0.5$ (short dashes), and $t/J\to\infty$ (long dashes). Contrary to its classical counterpart ($t/J=0$), this model does not present a percolation threshold for any finite t/J.

threshold, this quantum diluted model follows the usual scheme of phase transition in constrained systems[10] and the critical exponents become renormalized.

III. DISCUSSION AND CONCLUSIONS

In order to understand the absence of a percolation threshold for finite t, one must go through the concepts of statistical and quantum mixing of states. The statistical averages are performed by associating to each eigenstate of the system a Gibbs factor $e^{-\beta\Lambda_R}$, where Λ_R is the eigenvalue of $\mathcal{H}$ in the eigenstate R. In the present model, the bond configuration of any eigenstate is the direct product of the eigenstates of each bond,

$$|\Phi_R\rangle=\prod_i |\phi_{i,r}\rangle \ , \tag{9}$$

with the index i running over all lattice bonds and r standing for plus (+) or minus (−). For example, one single-bond eigenstate may be written as

$$|\phi_{i,r}\rangle=a_r|0\rangle+b_r|1\rangle \ , \tag{10}$$

where $a_\pm$ and $b_\pm$ can be obtained by standard matrix algebra. It is then clear that any eigenstate $|\Phi_R\rangle$ has components with the number of uncut bonds above the classical percolation threshold no matter what values a_r and b_r may take ($b_r\neq 0$). These components are actually responsible for the long-range ordering at $T=0$ for any $p\neq 0$. Another way to interpret this feature is by defining a bond strength operator $\hat{\mathbf{J}}$ with eigenvalues $\hat{\mathbf{J}}|0\rangle=0|0\rangle$ and $\hat{\mathbf{J}}|1\rangle=J|1\rangle$. In this way the average bond strength on eigenstate $|\phi_{i,r}\rangle$ is $\langle\phi_{i,r}|\hat{\mathbf{J}}|\phi_{i,r}\rangle=Jb_r^2$, so that each eigenstate has a finite and positive average bond strength and no percolation phenomenon shall appear. For $t/J\to\infty$, only the $|\phi_{i,-}\rangle$ states are relevant as $e^{-\beta(\lambda_+-\lambda_-)}\to 0$. In this limit $b_-^2(t/J\to\infty)=p$ and this explains the $T_c(t/J\to\infty)=pT_c(p=1)$ relationship, mentioned in the previous section. A more physical understanding of this limit can be achieved by noting that t actually defines the frequency at which the bond configuration is changing. As $t/J\to\infty$, the bond configuration changes so quickly that its strength is locally averaged and a standard local mean-field behavior shall then take place.

In conclusion, the phase diagram of an Ising model with annealed dilution, including a quantum mixing of states, is exactly obtained by using the decoration identities. The quantum mixing introduced is equivalent to considering that the bonds have a finite probability amplitude t of hopping to or from a bond reservoir. It is observed that the model has a quite distinct phase diagram when compared to its classical counterpart or even to models with only internal hopping amplitudes. The most remarkable feature is the absence of a percolation threshold at any dimension $d>d_l$, where d_l is the lower critical dimension of the corresponding pure model. Roughly speaking, one should expect $t\propto m^{-1}$, where m is the mass of the particle whose random intercalation activates the superexchange coupling between the vertex spins. For intercalation of heavy particles, as, for example, in surfaces with random ion adsorption, one may argue that $t/J\ll 1$, and the dilution may be well described classically. On the other hand, a finite hopping amplitude t should become relevant in systems with electron or hole doping.

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