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Effect of dilution on phase transitions in a transverse Ising model

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The effect of random bond (site) dilution on the phase transition of a three-dimensional transverse Ising model is studied by a cluster variation, along with perturbation expansion method. Complete phase diagrams in the temperature—concentration—transverse-field space are constructed for both the cases. The value of critical transverse field as a function of concentration, at zero temperature, exhibits a discontinuity at the critical value of concentration for the existence of phase transition, as conjectured by Harris. As is expected for the existence of a second-order phase transition, the static susceptibility diverges on the critical surface.

I. INTRODUCTION

The transverse Ising model (TIM) was introduced by de Gennes[1] as a pseudospin model for hydrogen-bonded ferroelectrics[2] like KH_2PO_4 (KDP). Since then, TIM has been useful as a model for various systems,[3] for example, cooperative Jahn-Teller systems[4] like $DyVO_4$ and induced magnetic systems.[5,6] In two or more dimensions TIM has a finite-temperature phase transition which can be depressed to zero temperature by increasing the transverse field to a critical value. The one-dimensional TIM at zero temperature is also critical at a critical value of the transverse field. The TIM therefore serves as a model of quantum-critical phenomena at zero temperature. It is also known that the quantum-critical behavior of the zero-temperature d-dimensional TIM as a function of the transverse field is the same as the temperature-dependent critical behavior of the $(d+1)$-dimensional Ising model.[6-12] Recent real-space renormalization-group calculations have reproduced these properties of TIM.[13-15] More recently, TIM has also been used in the meson-field theory[16] and in lattice-gauge theories.[11,17]

Recently there has been interest in the problem of disorder in the TIM, which may apply to DKDP-KDP (where DKDP represents deuterated KDP) mixed systems[18] and diluted vanadates.[19-21] Bond- and site-diluted TIM have been studied by Green's-function techniques using random-phase and coherent-potential (RPA-CPA) approximations and some theoretical inconsistencies have been observed.[22] An interesting feature of the diluted TIM was conjectured by Harris[23]—the critical transverse field as a function of concentration at zero temperature should display discontinuity at the percolation concentration. Earlier theoretical treatments of the diluted TIM, for example, series expansions[24] and CPA calculations,[25] and experiments[26] could not verify Harris's conjecture. Recent real-space renormalization-group calculations for a two-dimensional bond-diluted TIM (Refs. 27 and 28) at zero temperature could show the existence of this discontinuity as a result of two fixed points at the percolation threshold. More recently, dos Santos[29] performed real-space renormalization-group calculations for the complete phase diagram and critical surface of two-dimensional bond-diluted TIM on a square lattice and verified Harris's conjecture.

Real experimental situations, to which the diluted TIM can be applied, correspond generally to three-dimensional systems.[18,26,30] However, on the other hand, to the knowledge of the author, detailed calculations of the phase diagram and critical surface do not exist for a three-dimensional diluted TIM. The purpose of the present paper is to present a cluster variation-perturbation calculation of the phase diagram of three-dimensional bond- (site-) diluted TIM. We use a two-spin cluster variational method, equivalent to the methods which have been used for dilute Ising[31-33] and dilute Heisenberg models,[34,35] along with a perturbation expansion, which is valid near the transition temperature. Complete phase diagrams are constructed for a three-dimensional simple cubic lattice, both for bond- and site-diluted cases. A discontinuity in the critical transverse field as a function of concentration of bonds (sites) at zero temperature is observed at the critical concentration. It is the first time that a discontinuity as conjectured by Harris is being verified for a three-dimensional diluted transverse Ising model. The static susceptibility is found to diverge on the critical surface.

In Sec. II we present formal variation-perturbation theory for the TIM. Sections III and IV contain the application of the theoretical development of Sec. II to the bond- and site-diluted TIM, respectively, where we develop analytical expressions for the critical surface and static susceptibility of the system. Numerical calculations of phase diagrams and susceptibility are presented in Sec. V along with a discussion of results and conclusions.

II. TWO-SPIN CLUSTER THEORY FOR THE TRANSVERSE ISING MODEL

We consider the Hamiltonian

$$\mathcal{H} = -2\sum_{(ij)} J_{ij} S_i^z S_j^z - 2\sum_i B S_i^z - \sum_i \Gamma_i S_i^x \ , \qquad (1)$$

where S_i are the spin-$\frac{1}{2}$ operators, J_{ij} are the nearest-neighbor interactions, and B is an external uniform magnetic field which, if otherwise mentioned, will be considered to be zero. Γ_i is the transverse field. We introduce the spin-deviation operators σ_i as[34]

$$\sigma_i = \bar{S} - S_i^z \ , \qquad (2)$$

where $\bar{S}$ is the internal-field or molecular-field parameter which describes the long-range order. In general, in case of disordered systems $\bar{S}$ should be site dependent,[35] but in this section for simplicity and for treating the bond-diluted case in Sec. III we take $\bar{S}$ to be site independent. In terms of σ_i we can write

$$\mathcal{H} = -BN\bar{S} - 2\bar{S}^2 \sum_{(ij)} J_{ij} - \sum_i [B - 2\bar{S}J_i(0)]\sigma_i - \sum_i \Gamma_i S_i^x - 2\sum_{(ij)} J_{ij}\sigma_i\sigma_i \ , \qquad (3)$$

where $J_i(0) = \sum_j J_{ij}$. Now we divide the total Hamiltonian in two parts as

$$\mathcal{H}_1 = -BN\bar{S} - 2\bar{S}^2 \sum_{(ij)} J_{ij} - \sum_i \Gamma_i S_i^x - \sum_i [B - 2\bar{S}J_i(0)]\sigma_i \qquad (4)$$

and

$$V = -2\sum_{(ij)} J_{ij}\sigma_i\sigma_i \ . \qquad (5)$$

The averaged unperturbed energy is then given by

$$-\beta F_0 = \langle \ln \mathrm{Tr} \exp(-\beta\mathcal{H}_1)\rangle_c \ , \qquad (6)$$

where $\langle \cdots \rangle_c$ means average over all the configurations of disorder (bonds or sites). $\beta = (k_B T)^{-1}$, k_B being Boltzmann's constant and T the absolute temperature. The perturbed free energy F' can be written as

$$-\beta F' = -\beta F + \beta F_0 = \langle \ln\langle \exp(-\beta V)\rangle_{\mathcal{H}_1}\rangle_c \ , \qquad (7)$$

where

$$\langle \cdots \rangle_{\mathcal{H}_1} = \frac{\mathrm{Tr}[\cdots \exp(-\beta\mathcal{H}_1)]}{\mathrm{Tr}\exp(-\beta\mathcal{H}_1)} \ . \qquad (8)$$

In the two-spin cluster approximation,[34] we have for the perturbed free energy

$$-\beta F_2' = \sum_{(ij)} \langle \ln\langle \exp(-\beta\mathcal{H}_{ij})\rangle_{\mathcal{H}_1}\rangle_c \ , \qquad (9)$$

with the two-spin Hamiltonian

$$\mathcal{H}_{ij} = -2J_{ij}S_i^z S_j^z + 2J_{ij}\bar{S}(S_i^z + S_j^z) + 2J_{ij}\bar{S}^2 - (\Gamma_i S_i^x + \Gamma_j S_j^x) \ . \qquad (10)$$

Substituting Eqs. (4), (8), and (10) in Eq. (9), and adding the unperturbed free energy F_0, the total averaged free energy can be written as

$$-\beta F = -N(z-1)\langle \ln[\mathrm{Tr}\exp(-\beta\mathcal{H}_{\mathrm{I}})]\rangle_c + \frac{Nz}{2}\langle \ln[\mathrm{Tr}\exp(-\beta\mathcal{H}_{\mathrm{II}})]\rangle_c \ , \qquad (11)$$

where z is the number of nearest neighbors and N is the total number of sites. Hamiltonians $\mathcal{H}_{\mathrm{I}}$ and $\mathcal{H}_{\mathrm{II}}$ are given by

$$\mathcal{H}_{\mathrm{I}} = -[B + 2\bar{S}J_i(0)]S_i^z - \Gamma_i S_i^x \qquad (12)$$

and

$$\mathcal{H}_{\mathrm{II}} = -(2J_{ij}S_i^z S_j^z + \lambda_i S_i^z + \lambda_j S_j^z + \Gamma_i S_i^x + \Gamma_j S_j^x) \ , \qquad (13)$$

where

$$\lambda_i = B + 2\bar{S}[J_i(0) - J_{ij}] \ . \qquad (14)$$

In order to calculate the total averaged free energy we therefore need to calculate $\mathrm{Tr}\exp(-\beta\mathcal{H}_{\mathrm{I}})$ and $\mathrm{Tr}\exp(-\beta\mathcal{H}_{\mathrm{II}})$. As can been seen diagonalization of $\mathcal{H}_{\mathrm{I}}$ is simple and one can then directly calculate the unperturbed partition function

$$Z_{\mathrm{I}} = \mathrm{Tr}\exp(-\beta\mathcal{H}_{\mathrm{I}}) \ . \qquad (15)$$

The diagonalization of $\mathcal{H}_{\mathrm{II}}$ is not simple and therefore in order to evaluate the partition function

$$Z_{\mathrm{II}} = \mathrm{Tr}\exp(-\beta\mathcal{H}_{\mathrm{II}}) \qquad (16)$$

we develop a perturbation expansion near the phase transition temperature in powers of λ_i. Details of the perturbation expansion and evaluation of Z_{II} are given in the Appendix. Finally the averaged free energy F can be calculated by performing the configuration averaging in the expression

$$-\beta F=-N(z-1)\langle \ln Z_{\mathrm{I}}\rangle_c+\frac{Nz}{2}\langle \ln Z_{\mathrm{II}}\rangle_c \ . \tag{17}$$

III. BOND-DILUTED TIM

In this section we apply the theory of Sec. II to a bond-diluted TIM. In this case the single-spin partition function Z_{I} is found to be

$$Z_{\mathrm{I}}=2\cosh\{(\beta/2)[\Gamma^2+4\bar{S}^2J_i^2(0)]^{1/2}\} \ . \tag{18}$$

As can be seen from the Appendix the two-spin cluster partition function Z_{II} is written as a sum of two parts as

$$Z_{\mathrm{II}}=Z_0+Z_2 \ , \tag{19}$$

where Z_0 and Z_2 are given as

$$Z_0=2[\cosh(\beta R_{ij}/2)+\cosh(\beta J_{ij}/2)] \tag{20}$$

and

$$Z_2=\beta[(\lambda_i+\lambda_j)^2U(R_{ij};J_{ij})+(\lambda_i-\lambda_j)^2V(R_{ij};J_{ij})] \ , \tag{21}$$

where

$$U(R_{ij};J_{ij})=\frac{1}{4R_{ij}}\left[\frac{R_+}{R_-}[\exp(\beta R_{ij}/2)-\exp(\beta J_{ij}/2)]-\frac{R_-}{R_+}[\exp(-\beta R_{ij}/2)-\exp(\beta J_{ij}/2)]\right] , \tag{22a}$$

$$V(R_{ij};J_{ij})=\frac{\Gamma^2}{R_{ij}}\left[(R_+)^{-2}[\exp(\beta R_{ij}/2)-\exp(-\beta J_{ij}/2)]-(R_-)^{-2}[\exp(-\beta R_{ij}/2)-\exp(-\beta J_{ij}/2)]\right] , \tag{22b}$$

with $R_\pm=R_{ij}\pm J_{ij}$. For the bond-diluted case R_{ij} and λ_i are given by

$$R_{ij}=(J_{ij}^2+4\Gamma^2)^{1/2} \ ,$$
$$\lambda_i=2\bar{S}[J_i(0)-J_{ij}] \ . \tag{23}$$

The averaged free energy of the system can be obtained by substituting Eqs. (18)—(23) into Eq. (17) and performing the configuration averaging over the random distribution of bonds. However, we leave the averaging for later on and concentrate on the region near the phase transition. A self-consistent equation is obtained for the variational parameter $\bar{S}$ by minimizing the total free energy F with respect to $\bar{S}$. This leads to

$$\langle J_i^2(0)P^{-1}\tanh(P/2)\rangle_c=\frac{2z}{z-1}\langle (Z_{\mathrm{II}})^{-1}[(D_i+D_j)^2U(R_{ij};J_{ij})+(D_i-D_j)^2V(R_{ij};J_{ij})]\rangle_c \ , \tag{24a}$$

with

$$P=[\Gamma^2+4\bar{S}^2J_i^2(0)]^{1/2} \tag{24b}$$

and

$$D_i=J_i(0)-J_{ij} \ . \tag{24c}$$

Assuming that a second-order phase transition exists, as the transition temperature T_c $(=1/\beta_c k_B)$ is reached the internal field parameter $\bar{S}$ approaches zero. One can therefore obtain an equation for the critical surface simply by linearizing Eq. (24) in $\bar{S}$, which, for the critical surface in the temperature—transverse-field—concentration space, leads to

$$\frac{(z-1)}{2z\Gamma}\langle J_i^2(0)\rangle_c\tanh(\beta\Gamma/2)=\langle (Z_0)^{-1}(\{[J_i(0)-J_{ij}]^2+[J_j(0)-J_{ji}]^2\}[U(R_{ij};J_{ij})+V(R_{ij};J_{ij})]+\{2[J_i(0)-J_{ij}][J_j(0)-J_{ji}]\}[U(R_{ij};J_{ij})-V(R_{ij};J_{ij})])\rangle_c \ . \tag{25}$$

In order to perform configuration averaging, it should be kept in mind that $J_i(0)$, $J_j(0)$, and J_{ij} are dependent random variables. In the expressions, where J_{ij} does not appear along with $J_i(0)$ [as on the left-hand side of Eq. (25)], $J_i(0)$ can take one of the $z+1$ values, denoted by J_m,

$$J_m = mJ \quad (m=0,1,\ldots,z) \tag{26}$$

with a probability

$$P(J_m) = \frac{z!}{m!(z-m)!} x^m (1-x)^{z-m} , \tag{27}$$

where x is the concentration of magnetic bonds. On the other hand, in expressions where J_{ij} and $J_i(0)$ occur simultaneously, like on the right-hand side of Eq. (25), depending on the choice of J_{ij}, the distribution of $J_i(0)$ changes. For example, when $J_{ij}=J$, $J_i(0)$ takes the value

$$J_m = J + mJ \quad (m=0,1,\ldots,z-1) \tag{28}$$

with respective probabilities

$$P(J_m) = x \frac{(z-1)!}{m!(z-1-m)!} x^m (1-x)^{z-1-m} . \tag{29}$$

Using the above-discussed averaging procedure, we get the following relation which determines the critical surface of the bond-diluted TIM:

$$[2+(z-2)x]\frac{1}{\Gamma}\tanh(\beta\Gamma/2) = \frac{4}{Z_0(J)}\{[1+x(2z-3)]U(J)+(1-x)V(J)\} , \tag{30}$$

where $U(J)$, $V(J)$, and $Z_0(J)$ are $U(R_{ij};J_{ij})$, $V(R_{ij};J_{ij})$, and Z_0, respectively, with J_{ij} replaced by J. For a pure TIM ($x=1$) this gives

$$\frac{z}{z-1}\frac{1}{\Gamma}\tanh(\beta\Gamma/2) = \frac{8U(J)}{Z_0(J)} . \tag{31}$$

It can be seen from Eq. (30) that in the limit $\Gamma \to 0$, Eq. (30) leads to the constant-coupling—approximation result for the bond-diluted Ising model,[31,36] which is

$$x\tanh(\beta J/2) = \frac{1}{z-1} . \tag{32}$$

From this relation the well-known constant-coupling—approximation result for a pure Ising model ($x=1$) is recovered.[37] From Eq. (32) the critical concentration of bonds for the existence of phase transition in an Ising model turns out to be $x_c = 1/(z-1)$.

We shall now concentrate on the zero-temperature phase transition. Equation (30) can be simplified in the limit $T \to 0$, which leads to, for the transition line in the Γ-x plane at $T=0$,

$$4(R-1)(1-x)\alpha^3 + (R+1)^3[1+(2z-3)x]\alpha - R(R-1)(R+1)^2[2+(z-2)x] = 0 , \tag{33}$$

where $\alpha = \Gamma/J$ and $R=(1+4\alpha^2)^{1/2}$. With $x=1$, Eq. (33) leads to the following relation, which determines the critical transverse field for a pure TIM in the present approximation for the existence of phase transition at $T=0$,

$$2(z-1)\alpha - zR(R-1) = 0 . \tag{34}$$

In order to compare results of our theory with other existing results, we made calculation of the critical transverse field for a squared lattice ($z=4$) and found $\alpha_c = 3.334$, which should be compared with the series expansion result $\alpha_c = 3.04$. At $x=1/(z-1)$, which, in the present approximation, corresponds to critical concentration for the bond-diluted Ising model, we find that Eq. (33) has two different solutions for the critical transverse field α_c. One solution is $\alpha_c = 0$ and another is a finite nonzero real solution. This clearly shows the existence of a discontinuity in the value of the critical transverse field as a function of concentration at zero temperature for the critical value of concentration, which is in accordance with the Harris conjecture. Detailed numerical results for the complete phase diagram of a three-dimensional simple cubic lattice will be presented in Sec. V.

Finally, in this section we obtain the static susceptibility for the bond-diluted TIM. The averaged free energy F is a function of $\bar{S}$, which in turn depends on the external field B, taken to be finite to calculate the susceptibility. Therefore the magnetization M and susceptibility χ will be given by the relations

$$M = -\beta\frac{\partial F(B,\bar{S})}{\partial B} \tag{35}$$

and

$$\chi = \frac{dM(B,\bar{S})}{dB} = \frac{\partial M(B,\bar{S})}{\partial B} + \frac{\partial M(B,\bar{S})}{\partial \bar{S}}\frac{\partial \bar{S}}{\partial B} , \tag{36}$$

where the derivative $\partial\bar{S}/\partial B$ is to be determined from Eq. (24) in the presence of the external field B. As we are interested in the region near and above T_c (where $\bar{S}=0$), the calculation of the susceptibility χ is much simplified and we obtain

$$\frac{\chi}{\chi_0} = B(J,\Gamma,x,z) + \frac{z(z-1)x^2A^2(J,\Gamma)}{G(J,\Gamma,x,z)} , \tag{37}$$

where χ_0 is a constant and

$$A(J,\Gamma) = \frac{8U(J)}{Z_0(J)} - \frac{1}{\Gamma}\tanh(\beta\Gamma/2) , \tag{38}$$

$$B(J,\Gamma,x,z) = \frac{8zxU(J)}{Z_0(J)} - \frac{(zx-1)}{\Gamma}\tanh(\beta\Gamma/2) , \tag{39}$$

and

$$G(J,\Gamma,x,z)=[2+(z-2)x]\frac{1}{\Gamma}\tanh(\beta\Gamma/2) -\frac{4}{Z_0(J)}\{[1-(2z-3)x]U(J) +(1-x)V(J)\}\ . \qquad (40)$$

Comparing Eq. (40) with Eq. (30), which gives the critical surface in the T-Γ-x space, it can be easily seen that on the critical surface $G(J,\Gamma,x,z)=0$, which, in turn, with the use of Eq. (37), shows that susceptibility χ diverges on the critical surface, as is expected in case of a second-order phase transition. Detailed numerical results for χ will be given in Sec. V.

IV. SITE-DILUTED TIM

For the site-diluted TIM, in this section we use a slightly different approach. The Hamiltonian of the site-diluted TIM is assumed to be

$$\mathcal{H}=-2\sum_{(ij)}J_{ij}S_i^zS_j^zK_iK_j-2B\sum_i S_i^zK_i -\Gamma\sum_i S_i^xK_i\ , \qquad (41)$$

where the random numbers K_i take the values $K_i=1$ if the site i is occupied by a spin and $K_i=0$ if the site i is unoccupied, i.e., occupied by a nonmagnetic atom. Averaging K_i over all possible configurations $[K_i]$ gives the concentration x of spins, which is independent of the site index i, if the system is assumed to be homogeneously disordered. In the present case we introduce site-dependent internal-field parameters τ_i, which describe the long-range order and the fluctuating local fields for the disordered systems. Separating the Hamiltonian $\mathcal{H}$ in two parts, i.e., the single-spin part and the interaction part, as in Sec. II, we can develop a cluster expansion. Following the procedure of Hoeppener *et al.*[35] and the method of Sec. II, we can write the averaged free energy of the system in the two-spin cluster approximation as

$$-\beta F=\sum_{(ij)}[\ln\langle\exp(-\beta\mathcal{H}_{ij})\rangle_{\mathcal{H}'_{\rm I}}]_{K_i} +\sum_i[K_i\ln\Phi_1(\lambda_i;\Gamma)]_{K_i}\ , \qquad (42)$$

where the square brackets with subscript K_i denote averaging over all the configurations of K_i, and

$$\Phi_1(\lambda_i;\Gamma)={\rm Tr}\exp(-\beta\mathcal{H}'_{\rm I})\ , \qquad (43)$$

with

$$\mathcal{H}'_{\rm I}=-\lambda_iS_i^zK_i-\Gamma S_i^xK_i \qquad (44)$$

and

$$\lambda_i=2\sum_j J_{ij}\tau_j+2B\ . \qquad (45)$$

The two-spin Hamiltonian $\mathcal{H}_{ij}$ is given by

$$\mathcal{H}_{ij}=-(2J_{ij}S_i^zS_j^zK_iK_j-\tau_jS_i^zK_i-\tau_iS_j^zK_j)\ . \qquad (46)$$

As usual, considering only the nearest-neighbor interactions, we have $Nz/2$ different pairs of neighbors. It is easy to see that the contributions to free energy [Eq. (42)] F that come from pairs (i,j) where both sites are occupied by magnetic atoms can be separated from those coming from the pairs (i,j) where only one site is occupied by a spin. Applying these considerations and rearranging the terms in Eq. (42) we can write the averaged free energy in the two-spin cluster approximation

$$-\beta F_2=Nx[\ln\Phi_1(\lambda_i;\Gamma)]_{K_i}+\frac{Nz}{2}\{K_iK_j[\ln\Phi_2(\lambda_i-2J\tau_j,\lambda_j-2J\tau_i;\Gamma)-2\ln\Phi_1(\lambda_i;\Gamma)]\}_{K_i} +Nz\{K_i(1-K_j)[\ln\Phi_1(\lambda_i-2J\tau_j;\Gamma)-2\ln\Phi_1(\lambda_i;\Gamma)]\}_{K_i}\ , \qquad (47)$$

where

$$\Phi_2(\lambda_i,\lambda_j;\Gamma)={\rm Tr}\exp(-\beta\mathcal{H}'_{\rm II})\ , \qquad (48)$$

with

$$\mathcal{H}'_{\rm II}=-(2J_{ij}S_i^zS_j^z+\lambda_iS_i^z+\lambda_jS_j^z+\Gamma S_i^x+\Gamma S_j^x)\ . \qquad (49)$$

As in the bond-diluted case, $\mathcal{H}'_{\rm I}$ can be diagonalized easily and one can directly get $\Phi_1(\lambda_i;\Gamma)$. For calculating $\Phi_2(\lambda_i,\lambda_j;\Gamma)$, once again we note that the diagonalization of $\mathcal{H}'_{\rm II}$ is not simple and therefore we use the perturbation expansion in powers of λ_i, as discussed in Sec. II and described in Appendix. Once Φ_1 and Φ_2 are known, one has to perform the averaging over all the configurations of K_i. Here we use an approximation called the "first approximation" by Hoeppener *et al.*,[35] where we assume that τ_i does not depend on site i and put $\tau_i=x\bar{S}$. A more general approximation,[35] as in the case of a diluted Heisenberg model, with a site dependent τ_i may be expected to give better results. However, we checked, by explicit calculations, that in case of site-diluted TIM this other approximation does not change the general qualitative results appreciably. We therefore use the above-mentioned first approximation for averaging the free energy, which leads to

$$-\beta F_2=\tfrac{1}{2}Nzx^2\ln\Phi_2(2B+2J(z-1)x\bar{S},2B+2J(z-1)x\bar{S};\Gamma)$$
$$+Nzx(1-x)\ln\Phi_1(2B+2J(z-1)x\bar{S};\Gamma)-Nx(z-1)\ln\Phi_1(2B+2Jzx\bar{S};\Gamma)\ . \tag{50}$$

In the present case Φ_1 and Φ_2 are found to be

$$\Phi_1(\lambda;\Gamma)=2\cosh\{(\beta/2)[\Gamma^2+\lambda^2]^{1/2}\} \tag{51}$$

and

$$\Phi_2(\lambda,\lambda;\Gamma)=Z_0(J)+4\beta\lambda^2U(J)\ , \tag{52}$$

where $Z_0(J)$ and $U(J)$ are the same as defined earlier in Sec. III.

By minimizing the averaged free energy F_2 with respect to $\bar{S}$, a self-consistent equation for $\bar{S}$ is obtained as

$$\frac{(1-x)(z-1)}{L}\tanh(\beta L/2)-\frac{z}{K}\tanh(\beta K/2)+8x(z-1)U(J)[Z_0+16\beta x^2(z-1)^2J^2\bar{S}^2U(J)]^{-1}=0\ , \tag{53}$$

where

$$L=[\Gamma^2+4x^2(z-1)^2J^2\bar{S}^2]^{1/2}$$

and

$$K=[\Gamma^2+4x^2z^2J^2\bar{S}^2]^{1/2}\ .$$

Once again, as in the bond-diluted case, assuming the existence of a second-order phase transition, one can linearize Eq. (53) in $\bar{S}$ and can get the following relation which determines the critical surface of the site-diluted TIM:

$$(zx-x+1)\frac{1}{\Gamma}\tanh(\beta\Gamma/2)=8x(z-1)\frac{U(J)}{Z_0(J)}\ . \tag{54}$$

It can be verified easily that in case of a pure trans-

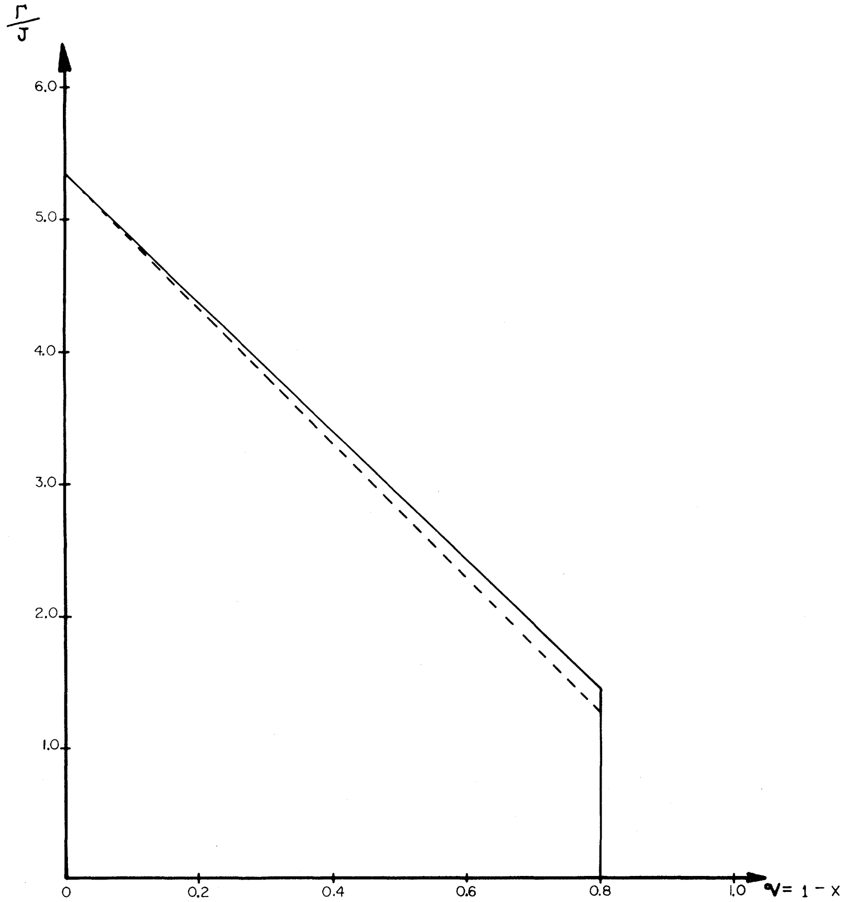

FIG. 1. Variation of critical transverse field ($\alpha=\Gamma/J$) as a function of $q=1-x$ (x being the concentration) at zero temperature for bond-diluted (——) and site-diluted (— — —) transverse Ising models.

verse Ising model ($x=1$) and in case of a site-diluted Ising model ($\Gamma=0$), Eq. (54) leads to the same behavior in the respective cases as obtained in Sec. III from the case of bond-diluted TIM.

Concentrating on the zero-temperature phase transition Eq. (54) simplifies, in the limit $T\rightarrow 0$, and gives the following relation for the transition line in Γ-x plane at $T=0$:

$$2x(z-1)(R+1)\alpha-(zx-x+1)R(R-1)=0\,. \tag{55}$$

For the pure TIM ($x=1$), as is expected, this leads to Eq. (34) for the critical transverse field at $T=0$.

As mentioned above, the behavior for $\Gamma=0$ is found to be the same as that obtained in the bond-diluted case, the critical concentration of spins in the case of site-diluted case also turns out to be $x_c=1/(z-1)$. Once again, considering the zero-temperature phase transition for this critical value of the concentration of spins, we find that Eq. (55) admits two different solutions for the critical transverse field, i.e., $\alpha_c=0$ and another finite solution, verifying a discontinuity in accordance with the Harris conjecture. Detailed numerical results and a complete phase diagram for a three-dimensional simple cubic lattice will be presented in Sec. V.

Finally the static susceptibility in the present case, following the procedure of Sec. III, is found to be

$$\frac{\chi}{\chi_0}=B(J,\Gamma,x,z)+\frac{z(z-1)x^2A^2(J,\Gamma)}{G_1(J,\Gamma,x,z)}\,, \tag{56}$$

where $B(J,\Gamma,x,z)$ and $A(J,\Gamma)$ are the same as defined in Sec. III and $G_1(J,\Gamma,x,z)$ is given by

$$\begin{aligned}G_1(J,\Gamma,x,z)=&\,(zx-x+1)\frac{1}{\Gamma}\tanh(\beta\Gamma/2)\\&-8x(z-1)\frac{U(J)}{Z_0(J)}\,.\end{aligned} \tag{57}$$

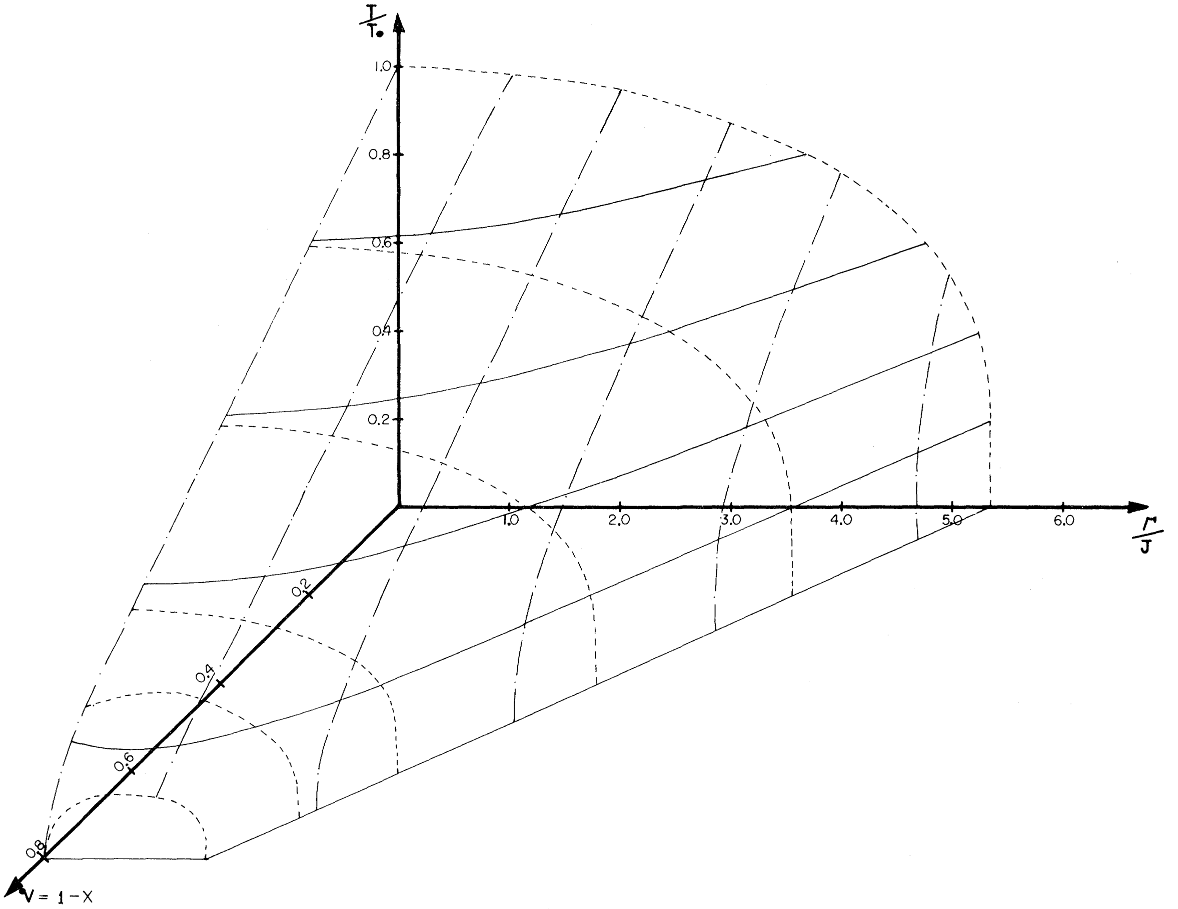

FIG. 2. Phase diagram of a bond-diluted transverse Ising model. Continuous lines (——) represent constant reduced-temperature (T/T_0) transition lines in the transverse-field ($\alpha=\Gamma/J$)—concentration ($x=1-q$) planes. Dashed lines (— — —) are the constant-x transition lines for the transition temperature (T/T_0) as a function of α. Dashed-dotted lines (—•—) represent constant-α transition lines for T/T_0 as a function of $q=(1-x)$.

As in the case of bond-diluted TIM, one can see that $G_1 = 0$ exactly corresponds to Eq. (54) determining the critical surface of the site-diluted TIM, which indicates that here also the static susceptibility diverges on the critical surface.

V. RESULTS AND DISCUSSION

In this section we present the numerical results and phase diagrams calculated on the basis of the theories of Secs. III and IV. First we consider the zero-temperature phase-transition line in the Γ-x plane as calculated from Eqs. (35) and (55) for the bond-diluted and site-diluted cases, respectively. Results for a three-dimensional simple cubic lattice ($z = 6$) are presented in Fig. 1, from which one can see that for $q = 1 - x_c = 0.8$, which corresponds to the critical concentration of a diluted Ising model on a simple cubic lattice in the present theory, the value of $\alpha = \Gamma/J$ shows discontinuity both for bond- and site-diluted TIM. However, the value of the discontinuity $\Delta\alpha(x_c)$ is found to be more for the bond-diluted case than for the site-diluted case. These results are in accordance with the Harris conjecture. In order to compare the results of our theory with other theories, we made calculations, based on Eqs. (33) and (55), of the discontinuity $\Delta\alpha(x_c)$ at the critical concentration for a two-dimensional square lattice ($z = 4$) and found

$$\Delta\alpha(x_c) = 1.419$$

for the bond-diluted TIM and

$$\Delta\alpha(x_c) = 1.277$$

for the site-diluted TIM. These values can be compared with $\Delta\alpha(x_c) = 1.746$ obtained for a bond-diluted TIM on a square lattice by real-space renormalization-group method.

In Figs. 2 and 3 we present complete phase diagrams for three-dimensional (simple-cubic-lattice) bond-diluted and site-diluted TIM's, respectively. As can be seen from these diagrams, the discontinuity in the critical transverse field at the critical concentration of bonds (sites) at zero temperature continues to exist at very low temperatures too. Fur-

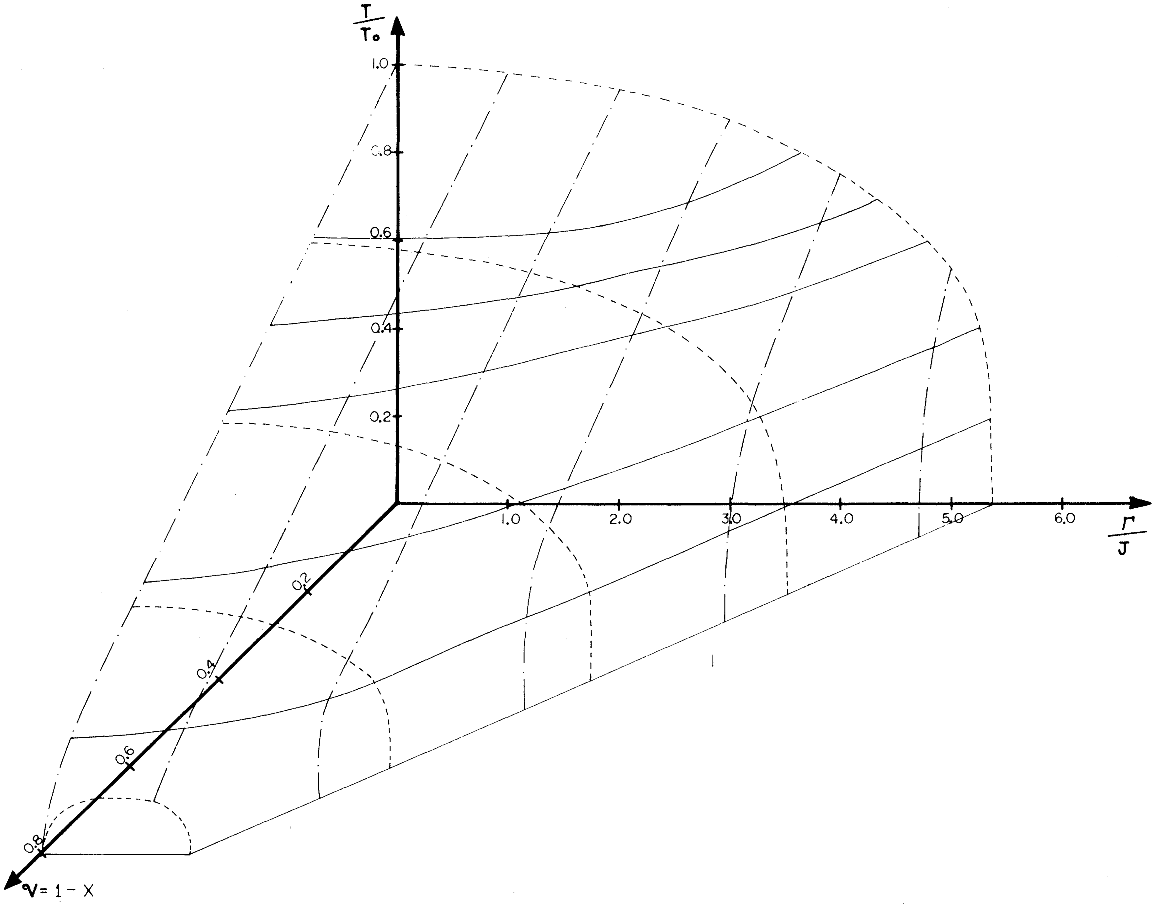

FIG. 3. Same as Fig. 2 for a site-diluted transverse Ising model.

ther, for lower transverse fields the critical temperature as a function of concentration also shows a discontinuity at the value of the critical concentration. One can see that the shpaes of the critical surfaces for both the cases, i.e., bond-diluted and site-diluted, are very similar. The only differences are in the values of discontinuities at the critical concentration. The phase diagrams of Figs. 2 and 3 can be compared with the real-space renormalization-group results[29] for the critical surface of a two-dimensional bond-diluted TIM on a square lattice. In this later case the only discontinuity is that in the critical transverse field at $T=0$ for the critical concentration. All other discontinuities observed in the present theory for a three-dimensional case are absent in the two-dimensional case mentioned above.

In Fig. 4 we present the inverse static susceptibility χ_0/χ as a function of temperature T/T_0 (T_0 be-

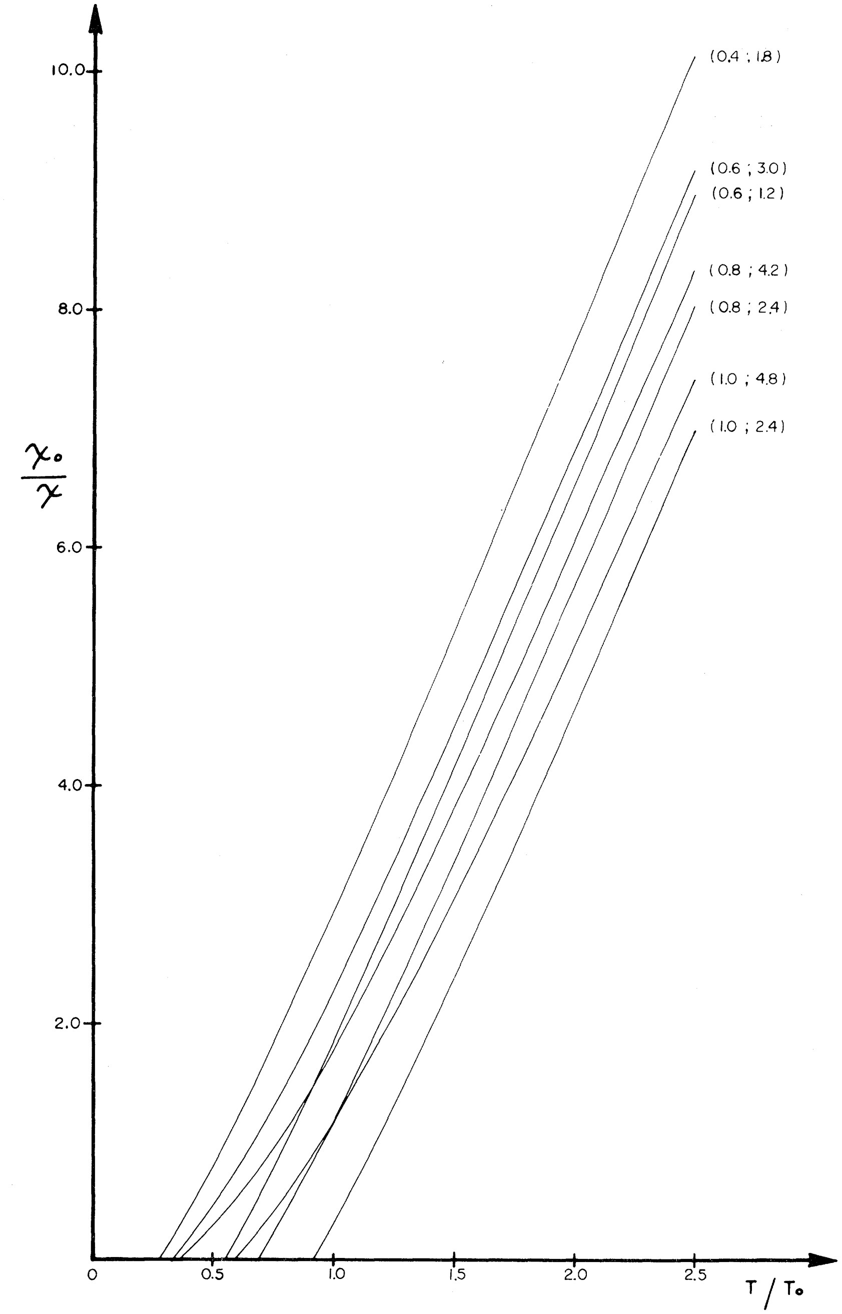

FIG. 4. Inverse static susceptibility χ_0/χ as a function of reduced temperature T/T_0 for various values of concentration (x) and transverse field ($\alpha=\Gamma/J$). Numbers in parentheses represent (x;α).

ing the critical temperature of a pure Ising model with $\Gamma=0$ in the present two-spin cluster approximation) for the bond-diluted TIM for various values of the concentration x and transverse field Γ. As can be seen in all the cases presented, χ_0/χ goes to zero, corresponding to the divergence of the susceptibility in case of second-order phase transitions. As the numerical results for χ_0/χ for the site-diluted TIM were found to be very similar to those presented in Fig. 4 for the bond-diluted case, we do not present the susceptibility curves separately for the site-diluted case. As can be seen the χ_0/χ-vs-T curves deviate much from linearity in the vicinity of T_c.

In conclusion, in this paper we used a two-spin cluster-variation method along with a second-order perturbation expansion valid near the phase transition to study the phase diagrams of three-dimensional bond-diluted and site-diluted Ising models in presence of a transverse field. A discontinuity in the critical transverse field as a function of concentration of bonds (sites) at the value of the critical concentration x_c at $T=0$, as conjectured by Harris,[23] was observed in both cases. To the best of our knowledge this is the first time that the discontinuity as conjectured by Harris has been observed for a three-dimensional diluted TIM. Whenever possible the results of the present theory have been compared with other existing theoretical results for similar systems, particularly the real-space renormalization-group calculations on a square lattice. We do not know of any experimental results which can be used to check the present results and which show the discontinuity conjectured by Harris. As is well known, the two-spin cluster approximation is a suitable approximation only at higher temperatures; the validity of the present results has limitations. However, qualitatively, the results are very reasonable and comparable to other existing theories, particularly verification of discontinuity conjectured by Harris for a three-dimensional case. A renormalization-group analysis of the phase transition and critical behavior of a three-dimensional diluted TIM is desirable in order to confirm and improve the results of the present theory.

APPENDIX

In this Appendix we calculate the two-spin partition function

$$Z_{\mathrm{II}}=\mathrm{Tr}\exp(-\beta\mathscr{H}_{\mathrm{II}})\ , \tag{A1}$$

with

$$\mathscr{H}_{\mathrm{II}}=-2J_{ij}S_i^zS_j^z-\lambda_iS_i^z-\lambda_jS_j^z-\Gamma(S_i^x+S_j^x)\ . \tag{A2}$$

We divide the Hamiltonian $\mathscr{H}_{\mathrm{II}}$ in two parts $\mathscr{H}_0$ and $\mathscr{H}_{\mathrm{I}}$ as

$$\mathscr{H}_0=-2J_{ij}S_i^zS_j^z-\Gamma(S_i^x+S_j^x) \tag{A3}$$

and

$$\mathscr{H}_{\mathrm{I}}=-\lambda_iS_i^z-\lambda_jS_j^z\ . \tag{A4}$$

$\mathscr{H}_0$ can be diagonalized easily and the eigenvalues and eigenvectors are found to be

$$\begin{aligned}
E_1&=-\frac{R_{ij}}{2}\ ,\quad |\Psi_1\rangle=(2P_{ij}^{+})^{-1}[(R_{ij}+J_{ij})(\,|++\rangle+|--\rangle)+2\Gamma(\,|+-\rangle+|-+\rangle)]\ ,\\
E_2&=-\frac{J_{ij}}{2}\ ,\quad |\Psi_2\rangle=(2)^{-1/2}(\,|++\rangle-|--\rangle)\ ,\\
E_3&=\frac{J_{ij}}{2}\ ,\quad |\Psi_3\rangle=(2)^{-1/2}(\,|-+\rangle-|+-\rangle)\ ,\\
E_4&=\frac{R_{ij}}{2}\ ,\quad |\Psi_4\rangle=(2P_{ij}^{-})^{-1}[(J_{ij}-R_{ij})(\,|++\rangle+|--\rangle)+2(\,|+-\rangle+|-+\rangle)]\ ,
\end{aligned} \tag{A5}$$

with

$$P_{ij}^{\pm}=[R_{ij}(R_{ij}\pm J_{ij})]^{1/2}$$

and

$$R_{ij}=(J_{ij}^2+4\Gamma^2)^{1/2}\ .$$

As we are interested in the behavior near the phase transition where the internal field parameter $\bar{S}$ and therefore the parameters λ_i are very small (in fact $\lambda_i\to 0$ as $T\to T_c$), we can safely develop a perturbation expansion in terms of the Hamiltonian $\mathscr{H}_{\mathrm{I}}$. Thus we write for Z_{II}

$$
\begin{aligned}
Z_{\mathrm{II}} &= \mathrm{Tr}\exp(-\beta\mathcal{H}_{\mathrm{II}}) = \mathrm{Tr}\exp[-\beta(\mathcal{H}_0+\mathcal{H}_{\mathrm{I}})] \\
&= \mathrm{Tr}\exp(-\beta\mathcal{H}_0) + \mathrm{Tr}\left[\sum_{n=1}^{\infty}(-1)^n \exp(-\beta\mathcal{H}_0)\right. \\
&\qquad\left. \times \int_0^{\beta} dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n \mathcal{H}_{\mathrm{I}}(t_1)\mathcal{H}_{\mathrm{I}}(t_2)\cdots\mathcal{H}_{\mathrm{I}}(t_n)\right] ,
\end{aligned}
\tag{A6}
$$

where

$$
\mathcal{H}_{\mathrm{I}}(t) = \exp(t\mathcal{H}_0)\mathcal{H}_{\mathrm{I}}\exp(-t\mathcal{H}_0) .
\tag{A7}
$$

Using the eigenvalues of the Hamiltonian $\mathcal{H}_0$ given in Eq. (A5), one can directly write, for $Z_0 = \mathrm{Tr}\exp(-\beta\mathcal{H}_0)$,

$$
Z_0 = 2\cosh(\beta R_{ij}/2) + 2\cosh(\beta J_{ij}/2) .
\tag{A8}
$$

It is easy to verify that the first-order term ($n=1$) in expansion (A6) vanishes. Therefore, since we are interested in the region near T_c where $\lambda_i \cong 0$, we look for the second-order terms only and neglect the higher-order terms in expansion (A6). The second-order term can be written as

$$
\begin{aligned}
Z_2 &= \mathrm{Tr}\left[\exp(-\beta\mathcal{H}_0)\int_0^{\beta} dt_1 \int_0^{t_1} dt_2 \mathcal{H}_{\mathrm{I}}(t_1)\mathcal{H}_{\mathrm{I}}(t_2)\right] \\
&= \sum_{k=1}^{4} \int_0^{\beta} dt_1 \int_0^{t_1} dt_2 \langle \Psi_k \mid \mathcal{H}_{\mathrm{I}}(t_1)\mathcal{H}_{\mathrm{I}}(t_2) \mid \Psi_k \rangle \exp(-\beta E_k) ,
\end{aligned}
\tag{A9}
$$

where $\mid \Psi_k \rangle$ are the eigenstates of $\mathcal{H}_0$ defined in Eqs. (A5). Substituting $\mathcal{H}_{\mathrm{I}}(t_n)$ from Eq. (A7) and rearranging the terms in Eq. (A9) one can perform integrations to give

$$
Z_2 = \beta \sum_{\substack{k=1 \\ k\neq m}}^{4} \sum_{m=1}^{4} \frac{\mid \langle \Psi_k \mid \mathcal{H}_{\mathrm{I}} \mid \Psi_m \rangle \mid^2}{(E_m - E_k)} \exp(-\beta E_k) .
\tag{A10}
$$

E_k are the eigenvalues of $\mathcal{H}_0$ given in Eq. (A5). Using the eigenvectors $\mid \Psi_k \rangle$ defined in Eqs. (A5) one can evaluate the matrix elements $\langle \Psi_k \mid \mathcal{H}_{\mathrm{I}} \mid \Psi_m \rangle$. Finally we get, for Z_2,

$$
Z_2 = \beta\{(\lambda_i^2+\lambda_j^2)[U(R_{ij};J_{ij}) + V(R_{ij};J_{ij})] + 2\lambda_i\lambda_j[U(R_{ij};J_{ij}) - V(R_{ij};J_{ij})]\} ,
\tag{A11}
$$

where

$$
U(R_{ij};J_{ij}) = \frac{1}{4R_{ij}}\left[\frac{R_+}{R_-}[\exp(\beta R_{ij}/2) - \exp(\beta J_{ij}/2)] - \frac{R_-}{R_+}[\exp(-\beta R_{ij}/2) - \exp(\beta J_{ij}/2)]\right]
\tag{A12}
$$

and

$$
V(R_{ij};J_{ij}) = \frac{\Gamma^2}{R_{ij}}\{(R_+)^{-2}[\exp(\beta R_{ij}/2) - \exp(-\beta J_{ij}/2)] - (R_-)^{-2}[\exp(-\beta R_{ij}/2) - \exp(-\beta J_{ij}/2)]\} .
\tag{A13}
$$

Finally Z_{II} can be calculated from the sum of the two terms $Z_{\mathrm{II}} = Z_0 + Z_2$. We use these results in Secs. III and IV for the bond-diluted and site-diluted cases, respectively.

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