Classical generalized constant-coupling method for geometrically frustrated magnets: Microscopic formulation and effect of perturbations beyond nearest-neighbor interactions

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The critical behavior of the pyrochlore lattice with nearest-neighbor (NN) interactions, next-nearest-neighbor (NNN) interactions, and site dilution by nonmagnetic impurities is studied within the framework of the microscopic formulation of the generalized constant-coupling method. In the paramagnetic regime, we recover all the results previously obtained in a more phenomenological way, which were shown to be in excellent agreement with Monte Carlo calculations for this lattice. In the absence of applied magnetic field, it is found that, for antiferromagnetic interactions, the equilibrium configuration is a noncollinear configuration in which the total magnetization of the unit is zero and the condition under which such an ordered state occurs is also obtained from the calculation. However, frustration inhibits the formation of such a state, and the system remains paramagnetic down to 0 K, if only nearest-neighbor interactions are taken into account, in agreement with the now generally accepted idea. NNN interactions, however, can stabilize a noncollinear ordered state, or ferromagnetic one, depending on the relation between NN and NNN interactions, in agreement with mean-field calculations, and the phase diagram is calculated. Finally, it is found that site dilution is not enough by itself to form such an ordered state.

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I. INTRODUCTION

The study of the magnetic ordering in geometrically frustrated antiferromagnets (GFAF's) with a pyrochlore lattice is not a new problem in condensed matter physics. However, there has been a renewed interest during recent years in this lattice, mainly because, experimentally, a rich phenomenology has been found at low temperatures and novel phases have been identified, even though this system is a relatively simple crystal.[1–3] To summarize a very long story, it is found that the susceptibility in materials belonging to this class exhibits a high-temperature phase in which it follows the Curie-Weiss (CW) law. Below the Curie-Weiss temperature, geometrical frustration inhibits the formation of a long-range-ordered (LRO) state, and the system remains paramagnetic, even though there are strong correlations between units. This phase is universally present in these systems, and it is called the cooperative paramagnetic phase. Finally, at a certain temperature T_f, which depends on the particular material and, usually, is well below the CW temperature, there appear nonuniversal phases: some of the systems remain paramagnetic down to the lowest temperature reached experimentally,[4] some of them exhibit noncollinear ordered states,[5,6] or even some of them form a spin glass state,[7–9] even though the amount of disorder in the structure is very small. It is thus easy to understand the amount of theoretical attention these systems have generated.[10–18]

In the simplest theoretical description of GFAF's, the spins on the lattice are regarded as Heisenberg spins with only nearest-neighbor (NN) interactions. In this picture, it is predicted that the nontrivial degeneracy of the ground state inhibits the formation of a LRO state, and the system remains paramagnetic down to zero temperature.[10] However, due to the presence of frustration, the NN exchange does not fix an energy scale in the problem, and any small perturbation can break the nontrivial degeneracy of the ground state and lead to some kind of ordered state. Therefore, it is especially important to incorporate these possible perturbations in any model that tries to explain the low-temperature phases of these systems. Examples of perturbations present in real systems are next-nearest-neighbor (NNN) interactions, small anisotropies, long-range dipole-dipole interaction, or dilution by nonmagnetic impurities, to cite some.

In a series of recent papers,[19–21] the present authors have generalized the well-known constant-coupling method of magnetism,[22,23] to deal with geometrically frustrated lattices, in both the classical and quantum cases, in the cooperative paramagnetic region. The magnetic properties calculated within the framework of the classical generalized constant-coupling (GCC) method were found to be in excellent agreement with Monte Carlo (MC) calculations for those same quantities,[11,24,25] for both the *kagomé* and pyrochlore lattices. The main idea behind this technique is very simple, and it is based in the experimental and numerical observation that correlations in GFAF's are always short ranged.[4,5,11,12,16,17] Therefore, in order to calculate any thermodynamic quantity, we can start by calculating the partition function of an isolated cluster with p spins and, later, add the interactions with the surrounding $p-1$ spins outside the cluster by means of an effective field which is fixed by a self-consistency condition. This, almost phenomenological, formulation of the method allows one to easily compute thermodynamic quantities, mainly the susceptibility, in the paramagnetic region, by using a single effective field to characterize all the interactions with spins outside the cluster. However, it is not very useful to study the critical properties of these systems when NN interactions are antiferromagnetic. The reason is very simple. It is now generally accepted that the ordered state of these GFAF, if any, is not a simple antiferromagnetic configuration, as in bipartite lattices, but a noncollinear (NC) one, in which the total spin momentum of the unit is identi-

cally zero.[10] Obviously, we cannot characterize such an ordered state by using a single order parameter fixed by a single effective field (EF). What is even worse, even we know that we have to introduce different order parameters for each of the spins in the cluster, and different EF for the neighboring spins outside the cluster, it is not easy to intuitively see how these EF enter into the expressions of the order parameters. Therefore, we need to go beyond the phenomenological formulation of the GCC method introduced in the aforementioned works. This is precisely the intention of this work. We have constructed the GCC method from first principles by using rigorous identities in terms of averages over finite-size clusters. In this way, the EF naturally emerge as averages over the microscopic spin variables. This microscopic formulation of the GCC method not only allows us to recover all the results obtained Refs. 19 and 21 in the paramagnetic regime but, also, gives us the possible ordered configurations of the system and the conditions for a transition to one of these states to occur. Moreover, as the GCC method is constructed in the real space, it is especially easy to include further perturbations in the system. Particularly, we have studied the effect of NNN interactions and site dilution by nonmagnetic impurities. In the present work, we will only present the main results we have found in this framework for the critical properties of the pyrochlore lattice. A more detailed presentation of the method and the results for other frustrated lattices will be published elsewhere.[26]

II. SUSCEPTIBILITY AND CRITICAL BEHAVIOR IN THE FRAMEWORK OF THE GCC METHOD

As stated above, the original formulation of the GCC method[19,20] is not well suited to study the critical behavior of GFAF. Indeed, it is now generally accepted that the ground state of the pyrochlore and *kagomé* lattices is fixed by the condition that the total spin momentum of the tetrahedral or triangular unit, respectively, is zero, though frustration inhibits the formation of such a state and the system remains paramagnetic in the whole temperature range if only NN interactions are present. Obviously, we cannot characterize such an ordered state with a single order parameter, as we did in Refs. 19 and 20, which restricts the applicability of the GCC method to the study of the paramagnetic region or, at most, the ferromagnetic case, which is of less interest, due to the absence of geometrical frustration. A relatively simple way of circumventing this shortcoming of the method has been pointed out in Refs. 10 and 27, and essentially consists of introducing different sublattices characterized by different order parameters. The minimum number of sublattices we need to introduce is given by the number of spins in the cluster, that is, 3 and 4 for the *kagomé* and pyrochlore lattices, respectively (see Fig. 1). With this subdivision, spins belonging to one sublattice only interact with spins belonging to different sublattices. Therefore, the dimensionless Heisenberg Hamiltonian of a lattice formed by corner sharing clusters with p spins, and NN and NNN interactions, in the presence of a uniform magnetic field, can be put in the form

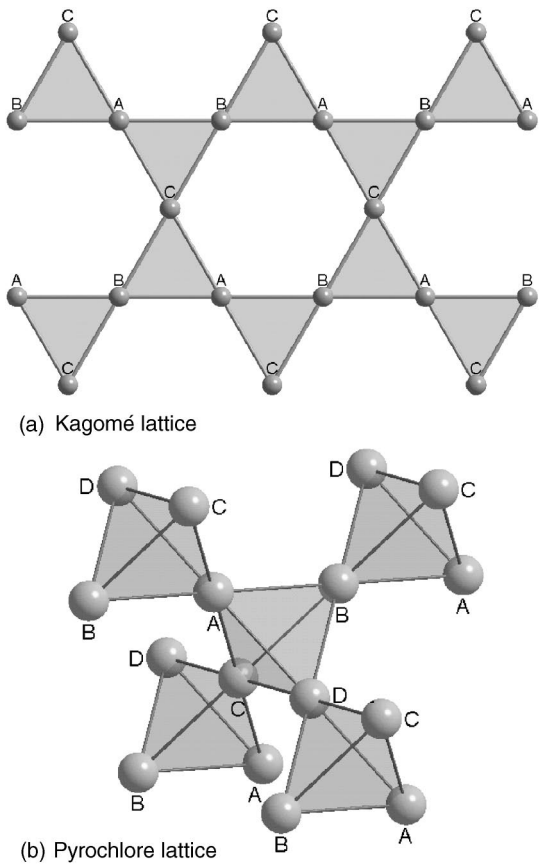

FIG. 1. Examples of highly frustrated lattices. $A,B,C,\ldots$ denote the sublattices in which the whole lattice is subdivided. All these lattices share the following property: if we consider a spin inside a cluster formed by p spins, there are $p-1$ NN spins outside the cluster. Notice also that one spin belonging to one sublattice does not have NN belonging to the same sublattice.

$$\mathcal{H}=K_1\sum_{\alpha\neq\beta}\sum_{\langle i,j\rangle}\vec{s}_{i\alpha}\cdot\vec{s}_{j\beta}+K_2\sum_{\alpha\neq\beta}\sum_{\langle\langle i,j\rangle\rangle}\vec{s}_{i\alpha}\cdot\vec{s}_{j\beta}+\vec{H}_0\cdot\sum_{\alpha,i}\vec{s}_{i\alpha}, \tag{1}$$

where $\vec{s}_{i\alpha}$ are the classical Heisenberg spins of unit length. The α index labels the sublattice to which the considered spin belongs (and takes the values $\alpha=A,B,C,\ldots$), whereas the i index labels the spins belonging to a given sublattice. $\langle\cdots\rangle$ represents sum over NN pairs, whereas $\langle\langle\cdots\rangle\rangle$ stands for sum over NNN pairs, $K_1=J_1/T$ ($K>0$ for ferromagnetic interactions and $K<0$ for antiferromagnetic ones) is the dimensionless NN exchange interaction, and $K_2=J_2/T$ is the dimensionless NNN exchange interaction. Finally, $\vec{H}_0=\vec{h}_0/T$, with $\vec{h}_0$ the applied magnetic field.

The central idea of the GCC method is to calculate the order parameter (for each sublattice) for two clusters of different sizes, p and p', replacing the effect of the spins not included in the cluster (NN and NNN) by fixed effective fields, which act as a symmetry breaking field (SBF) and, by using the self-consistency condition

$$\vec{m}_{p'\alpha}(K)=\vec{m}_{p\alpha}(K), \tag{2}$$

obtain an equation to determine these effective fields and, thus, the magnetization. The order parameter is calculated by making use of the Callen-Suzuki identity[28,27]

$$\vec{m}_{p\alpha}=\langle\vec{s}_{i\alpha}\rangle=\left\langle\frac{\mathrm{Tr}_p\vec{s}_{i\alpha}e^{\mathcal{H}_p}}{\mathrm{Tr}_p e^{\mathcal{H}_p}}\right\rangle_{\mathcal{H}}, \tag{3}$$

where the partial trace is taken over the set of p variables specified by the finite-size cluster Hamiltonian $\mathcal{H}_p$ and $\langle\cdots\rangle_{\mathcal{H}}$ indicates the usual canonical thermal average over the ensemble defined by the complete Hamiltonian $\mathcal{H}$.

The Hamiltonian of a one-spin cluster in sublattice α can be cast in the form

$$\mathcal{H}_{1\alpha}=\vec{s}_{1\alpha}\cdot\vec{\xi}_{1\alpha}, \tag{4}$$

where the subindex 1α makes reference to the fact that the Hamiltonian corresponds to a cluster of one spin belonging to sublattice α, and $\vec{\xi}_{1\alpha}$ stands for the symmetry breaking field acting on the spin of the one-spin cluster, which belongs to sublattice α. The expression for this SBF when both NN and NNN interactions are taken into account is given by

$$\vec{\xi}_{1\alpha}=\vec{H}_0+K_1\sum_{\beta\neq\alpha}\sum_{i}^{z}\vec{s}_{i\beta}+K_2\sum_{\beta\neq\alpha}\sum_{i}^{z'}\vec{s}_{i\beta}, \tag{5}$$

where z is the number of NN on each sublattice, z' stands for the number of NNN on each sublattice ($z'=4$ for the pyrochlore lattice). The order parameter for this cluster can be trivially evaluated by using Eq. (3), and near a critical point can be put, up to first order in the SBF, as

$$\vec{m}_{1\alpha}\simeq\frac{\langle\vec{\xi}_{1\alpha}\rangle_{\mathcal{H}}}{3}. \tag{6}$$

By defining the effective fields $\vec{h}'_\alpha=J_1\langle\vec{s}_{i\alpha}\rangle_{\mathcal{H}}=J_1\langle\vec{s}_{j\alpha}\rangle_{\mathcal{H}}$ $(i,j\neq 1)$, we arrive at the final expression for the order parameter for sublattice α of the one-spin cluster:

$$\vec{m}_{1\alpha}=\frac{1}{3|J_1|\tilde{T}}\left[\vec{h}_0+2(1+z'\lambda)\sum_{\beta\neq\alpha}\vec{h}'_\beta\right], \tag{7}$$

where $\lambda=J_2/J_1$, $\tilde{T}=1/|K_1|=T/|J_1|$, and we have taken into account that each spin has two NN on each sublattice different from the considered one.

With some more effort, we can also calculate the order parameter for a cluster with p atoms. Up to first order in the SBF, this quantity is given by

$$\vec{m}_{p\alpha}=\frac{\langle\vec{\xi}_{p\alpha}\rangle}{3}-\frac{z_p^1(K_1)}{3z_p^0(K_1)}\sum_{\beta\neq\alpha}\langle\vec{\xi}_{p\beta}\rangle, \tag{8}$$

where the SBF are now given by

$$\vec{\xi}_{p\alpha}=\vec{H}_0+K_1\sum_{\beta\neq\alpha}\sum_{i}^{z-1}\vec{s}_{i\beta}+K_2\sum_{\beta\neq\alpha}\sum_{i}^{z'}\vec{s}_{i\beta}, \tag{9}$$

and we have introduced the functions

$$z_p^0(K)=\int_0^\infty dq\,q^2e^{q^2/2K}\left(\frac{\sin q}{q}\right)^p \tag{10}$$

and

$$z_p^1(K)=\int_0^\infty dq\,q^2\,e^{q^2/2K}\left(\frac{\sin q}{q}\right)^{p-2}\left(\frac{\cos q}{q}-\frac{\sin q}{q^2}\right)^2. \tag{11}$$

Incidentally, the first term in Eq. (10) corresponds to the partition function for noninteracting clusters with no applied field, which were first calculated by Moessner and Berlinsky.[11] The additional terms $z_p^1(K)$ allow us to study not only the paramagnetic regime, but also the behavior of the system near a critical point, as we will see below.

Taking into account the definition of the SBF and the fact that $J_1\langle\vec{s}_{i\alpha}\rangle_{\mathcal{H}}=J_1\langle\vec{s}_{j\alpha}\rangle_{\mathcal{H}}=\vec{h}'_\alpha$, after some algebra we arrive at

$$\vec{m}_{p\alpha}=\frac{1}{3|J_1|\tilde{T}}\Big\{[1-(p-1)A_p(\tilde{T})]\vec{h}_0+[1-(1+z'\lambda)(p-2)A_p(\tilde{T})]\sum_{\beta\neq\alpha}\vec{h}'_\beta-(1+z'\lambda)(p-1)A_p(\tilde{T})\vec{h}'_\alpha\Big\} \tag{12}$$

where we have introduced the function $A_p(\tilde{T})=z_p^1(-\tilde{T})/z_p^0(-\tilde{T})$ for antiferromagnetic interactions. By direct substitution, it is simple to verify the relation

$$\varepsilon_p(\tilde{T})=-(p-1)A_p(\tilde{T}), \tag{13}$$

where $\varepsilon_p(\tilde{T})$ is defined as[19]

$$\varepsilon_p(\tilde{T})=\frac{2\tilde{T}^2}{p}\frac{\partial}{\partial\tilde{T}}\ln z_p^0(\tilde{T})-1. \tag{14}$$

Substituting Eqs. (12) and (7) into Eq. (2) we arrive at the following system of linear equations in the effective fields $\vec{h}_\alpha$:

$$-(1+z'\lambda)\varepsilon_p(\tilde{T})\vec{h}'_\alpha+\left[1-(1+z'\lambda)\frac{(p-2)}{(p-1)}\varepsilon_p(\tilde{T})\right]\sum_{\beta\neq\alpha}\vec{h}'_\beta=\varepsilon_p(\tilde{T})\vec{h}_0, \tag{15}$$

and its solution is given by

$$\vec{h}'_\alpha=\frac{\varepsilon_p(\tilde{T})}{(p-1)[1-(1+z'\lambda)\varepsilon_p(\tilde{T})]}\vec{h}_0. \tag{16}$$

Substituting back into the expression of the one-spin cluster order parameter we find the expression for the susceptibility:

$$\chi_p^{gcc}=\frac{1}{3|J_1|\tilde{T}}\frac{1+\varepsilon_p(\tilde{T})}{1-(1+z'\lambda)\varepsilon_p(\tilde{T})}. \tag{17}$$

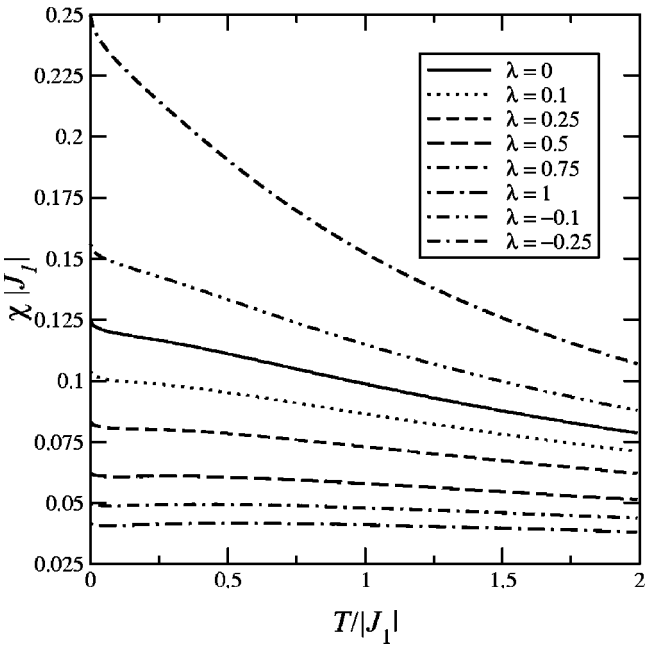

FIG. 2. Effect of NNN interactions on the susceptibility of the pyrochlore lattice.

This susceptibility is depicted in Fig. 2 for different values of λ and antiferromagnetic NN interactions.

In the absence of an applied field, the system (15) has two nontrivial solutions: the first one occurs if

$$\varepsilon_p(\tilde{T}) = -\frac{(p-1)}{1+z'\lambda} \tag{18}$$

and corresponds to an ordered state in which

$$\sum_{\alpha} \vec{m}_{\alpha} = \vec{0}. \tag{19}$$

We will call this kind of state a NC ordered state. Actually, this condition includes, as particular cases, states in which spins in different sublattices are antiferromagnetically aligned with each other, that is, collinear states. However, the most general state described by this condition is a noncollinear one. The second solution of Eq. (15) occurs if

$$\varepsilon_p(\tilde{T}) = \frac{1}{(1+z'\lambda)} \tag{20}$$

and corresponds to an ordered state in which

$$\vec{m}_{\alpha} = \vec{m}_{\beta} = \vec{m}_{\gamma} = \cdots \quad \forall \alpha, \beta, \gamma, \ldots, \tag{21}$$

that is, ferromagnetic order.

We will postpone the analysis of the critical behavior until the effects of dilution by nonmagnetic impurities are introduced in the next section.

III. EFFECT OF DILUTION BY NONMAGNETIC IMPURITIES

So far, nothing has been said about dilution by nonmagnetic impurities. In order to add this effect we need to average the order parameters and SBF over the distribution of nonmagnetic impurities. For simplicity, we will assume that the distribution of nonmagnetic impurities is purely random. Under this condition, the number of units with q spins, for a lattice which, in the absence of dilution, is formed by units with p spins, for a concentration of nonmagnetic impurities, x, is given by[11]

$$P_q^p(x) = \binom{p}{q} (1-x)^q x^{p-q}. \tag{22}$$

However, this distribution is normalized with respect to units, whereas we need a distribution function normalized with respect to a single spin. The adequate distribution function, for the SBF, is then given by

$$\mathcal{P}_p^p(x) = \frac{q}{p(1-x)} P_q^p(x), \tag{23}$$

whereas the corresponding one for the order parameter is given by

$$\mathcal{Q}_q^p(x) = (1-x)(q-1)\mathcal{P}_q^p(x). \tag{24}$$

In the following, we will use the following notation to denote averages with respect to dilution:

$$[f_q]_p = \sum_{q=1}^{p} \mathcal{P}_q^p(x) f_q, \tag{25}$$

where f_q is any quantity, and it will be understood that we are using the distribution (23) when averaging over SBF and the distribution (24) when averaging over the order parameter.

Therefore, if we construct the average over dilution of the self-consistency condition (2), i.e.,

$$[\vec{m}_{1\alpha}]_p = [\vec{m}_{q\alpha}]_p, \tag{26}$$

and follow the same steps as in the previous section, we easily arrive at an expression for the averaged susceptibility in the paramagnetic region:

$$[\chi]_p = \frac{1-x}{3|J_1|\tilde{T}} \frac{1+\overline{\varepsilon}_p}{1-(1+z'\lambda)\overline{\varepsilon}_p}. \tag{27}$$

In this expression,

$$\overline{\varepsilon}_p = \frac{2\tilde{T}^2}{p(1-x)} \frac{\partial}{\partial \tilde{T}} \ln \overline{z_p^0}(\tilde{T},x) - 1, \tag{28}$$

where $\overline{z_p^0}$ is the average of z_p^0 with respect to dilution, given by[21]

$$\overline{z_p^0} = \prod_{q=1}^{p} z_p^0(\tilde{T})^{P_q^p(x)}. \tag{29}$$

In the absence of an applied magnetic field, the condition for the existence of a ferromagnetic ordered state is very easily obtained to be[26]

$$\overline{\varepsilon}_p = \frac{1}{1+z'\lambda}, \tag{30}$$

whereas the corresponding one for a noncollinear ordered state is given by

$$\overline{\varepsilon}_p = -\frac{(p-1)(1-x)}{1+z'\lambda}. \tag{31}$$

These conditions have been studied for different values of x and the ratio between NN and NNN interactions, and the corresponding phase diagrams are depicted in Fig. 3. Also, in Fig. 4 we have depicted the values of $\lambda_c(x)$, that is, the value of J_2/J_1 above which a noncollinear ordered state is formed at a finite temperature, for a given value of x. We have only depicted this quantity for antiferromagnetic NN interactions, as the corresponding λ_c for ferromagnetic NN interactions does not change upon dilution.

Let us first discuss the phase diagram for the nondiluted case ($x=0$). As we can see from Fig. 3, NNN interactions can stabilize different ordered states depending on the value of λ and the sign of the NN interaction. For antiferromagnetic NN interactions and $|J_2|<0.5|J_1|$, the system remains paramagnetic down to 0 K. For antiferromagnetic NN and NNN interactions, a NC ordered state is selected at finite temperature for $\lambda>\frac{1}{2}$. However, for antiferromagnetic NN interactions and ferromagnetic NNN interactions, a ferromagnetic ordered state is selected for $\lambda<-\frac{1}{2}$. On the other hand, the case of ferromagnetic NN interactions is slightly more complex. For ferromagnetic NNN interactions, a ferromagnetic ordered state is selected for $-\frac{1}{6}<\lambda$. In the range $-\frac{1}{2}<\lambda<-\frac{1}{6}$, the system remains paramagnetic down to 0 K and, in the range $\lambda<-\frac{1}{2}$, a NC ordered state is selected. In any case, from the analysis of this section, it seems very unlikely that the noncollinear ordered states experimentally found in some pyrochlore systems are due to NNN interactions,[5,29] as in real pyrochlore systems $|J_2|\sim 0.1|J_1|$, a value well inside the region of the phase diagram in which the system is found to remain paramagnetic down to 0 K. It is also important to stress that the present treatment of NNN interactions is only approximate, and it does not contradict in any way previously published results in which is shown that NNN interactions could stabilize some kind of incommensurate state.[5,10] In fact, in order to treat this problem consistently, we should include new sublattices in such a way that spins in one sublattice do not interact with spins in the same sublattice. In doing so, it can happen that new kinds of ordered states arise, even in regions where our present simplified analysis predicts the system to remain paramagnetic. However, our main intention here is to check if the NC state given is selected by NNN interactions. The general problem with more sublattices will be studied elsewhere.

If we now turn our attention to the effect of dilution on the phase diagram, we can easily see that dilution by itself cannot induce a NC ordered state: the system remains paramagnetic for all values of x if $\lambda=0$, in contrast with the qualitative picture suggested in other works. The main effect of dilution seems to be to increase the transition temperature to a NC ordered state while decreasing the transition temperature to a ferromagnetic state for $J_1<0$, whereas the trend is exactly the opposite for $J_1>0$.

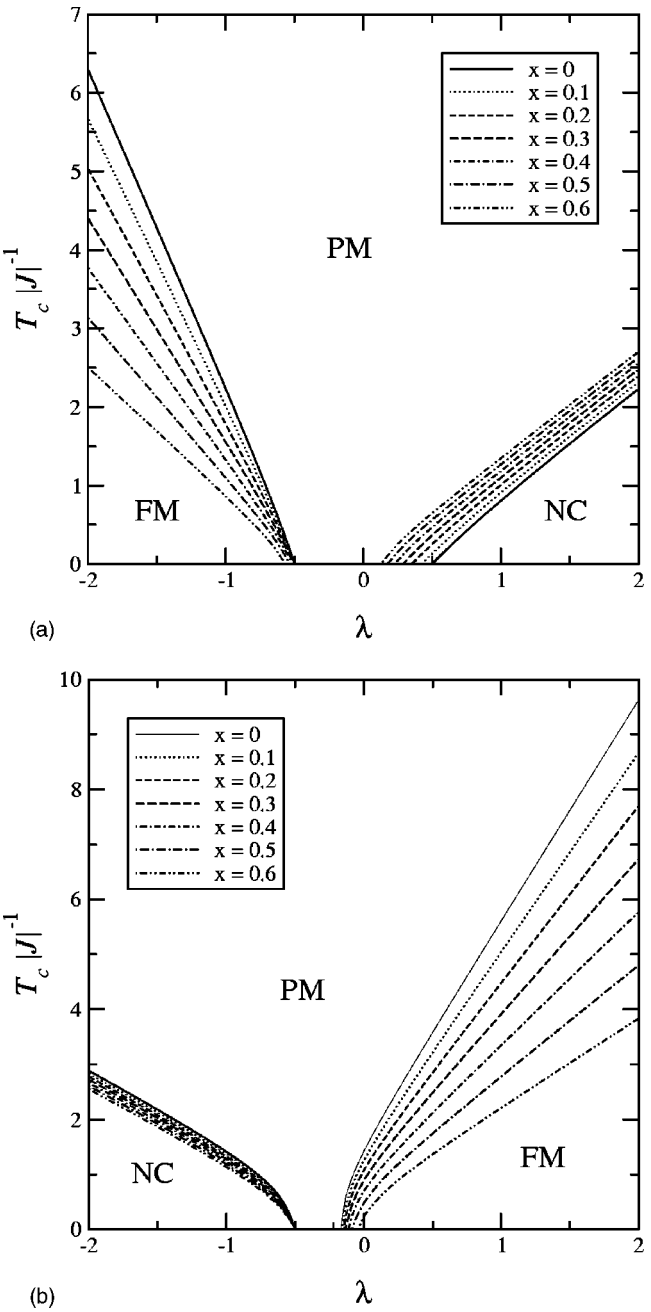

FIG. 3. Phase diagrams with both NNN interactions and site dilution. In these figures, FM stands for ferromagnetic order, PM for paramagnetic phase, and NC for noncollinear order.

IV. CONCLUSIONS

In this work we have presented the main results emerging from the microscopic formulation of the generalized constant-coupling method for classical Heisenberg spins in

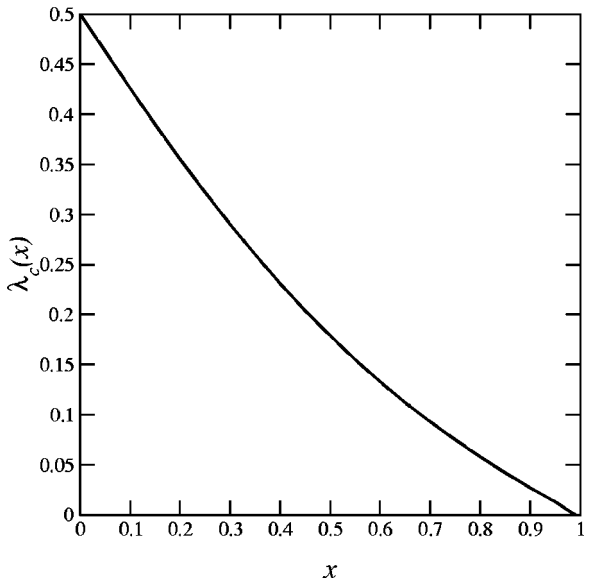

FIG. 4. Minimum value of λ for which a NC ordered state is formed for different concentrations of nonmagnetic impurities.

the presence of NN interactions, NNN interactions, and dilution by nonmagnetic impurities and how these effects affect the critical properties of geometrically frustrated magnets with a pyrochlore lattice.

When a magnetic field is applied to the system, this method allows us to easily compute the averaged susceptibility, and we recover previous results obtained in the phenomenological formulation of the GCC method, which were shown to be in excellent agreement with MC results for both the *kagomé* and pyrochlore lattice. However, the present formulation allows us to also study the critical behavior of the system when no applied magnetic field is present. One advantage of the present formulation is that it is constructed in real space, which makes it very easy to include additional perturbations to the system beyond NN interactions. Particularly, we have studied the effect of next-nearest-neighbor interactions and site dilution by nonmagnetic impurities for the pyrochlore lattice. The phase diagrams have been calculated. It is found that, for certain values of the ratio $\lambda = J_2/J_1$, a noncollinear or ferromagnetic ordered state can be stabilized. However, the minimum value of λ above which a noncollinear configuration is stable, for any concentration of nonmagnetic impurities, seems to be too large to explain the formation of long-range order found in some systems, notably in $Gd_2Ti_2O_7$.[5] Besides, the main perturbation in this system seems to come from long-range dipolar interactions, which are highly anisotropic. Further theoretical work in this direction, in the present framework, is still necessary.

Regarding the effects of site dilution, it has been argued that this kind of effect, always present in real materials, could break the nontrivial degeneracy of the ground state and cause a transition to some kind of long-range-ordered state at finite temperature. However, in our calculation, we find that this is not the case: Site dilution by itself does not induce a transition, for any amount of dilution. It is necessary to include simultaneously both dilution and next-nearest-neighbor interactions.

A word of caution must be said here, however. In the last part of this work, we have focused our attention on studying if a noncollinear ordered state given by the rule that the total magnetization of the tetrahedral unit is zero is estabilized by any of these perturbations. However, these are not the only possible ordered configurations when we include these effects. For example, Reimers and co-workers[10] showed that, in the framework of mean-field theory, next-nearest-neighbor interactions can induce both noncollinear ordered states as the ones studied in this work or ordered states characterized by an incommensurate wave vector. It is not easy to describe these incommensurate states with a real space method, and it could be the case that site dilution would lead to such an incommensurate state. Therefore, more theoretical work in that direction should be necesary before ruling out the possibility of a long-range-ordered state induced by small amounts of site dilution or—what would be even more interesting—the possibility of a transition to some kind of spin glass state induced by dilution.

In conclusion, the formulation of the generalized constant-coupling method presented in this work provides us a conceptual framework in which both thermodynamic quantities and the critical behavior of geometrically frustrated magnets can be properly described. The method can be easily generalized to deal with further perturbations always present in real systems. We have presented the classical limit of the method. However, in order to compare the calculated quantities with experimental data for these systems, the corresponding quantum generalized constant coupling method should be used. This issue, the occurrence of incommensurate states due to dilution, and the effect of the inclusion of long-range dipolar interactions in the Hamiltonian are open issues which deserve further theoretical work.

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