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Destruction of first-order phase transition in a random-field Ising model

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Abstract

The phase transitions that occur in an infinite-range-interaction Ising ferromagnet in the presence of a double Gaussian random magnetic field are analyzed. Such random fields are defined as a superposition of two Gaussian distributions, presenting the same width σ . It is argued that this distribution is more appropriate for a theoretical description of real systems than other simpler cases, i.e. the bimodal ($\sigma = 0$) and single Gaussian distributions. It is shown that a low-temperature first-order phase transition may be destroyed for increasing values of σ , similarly to what happens in the compound $\text{Fe}_x\text{Mg}_{1-x}\text{Cl}_2$, whose finite-temperature first-order phase transition is presumably destroyed by an increase in the field randomness.

1. Introduction

The theory of continuous phase transitions is very well established nowadays [1–3]. These transitions are characterized by a divergence of the correlation length in such a way that some microscopic details of the system become irrelevant, leading to the concept of universality classes for the critical exponents. Although first-order phase transitions are very common in nature, they have attracted much less attention from the theoretical point of view. In particular, the correlation length remains finite at such transitions and so a universal behavior is not expected. Many interesting features occur in first-order phase transitions, such as a discontinuity in the order parameter and the presence of latent heat. In addition to these, in some systems, it is possible for a first-order phase transition to become continuous due to changes in an external parameter or to the presence of microscopic inhomogeneities that may generate significant roundings in the transition [4]. Therefore, one important question concerns the effects of random quenched impurities on the thermodynamic phase transition.

The random-field Ising model (RFIM) was introduced by Imry and Ma [5] and has attracted a lot of interest after the identification of its physical realizations. Probably the most important physical concept of the RFIM is the diluted Ising antiferromagnet in the presence of a uniform magnetic field [6, 7]. In these systems one has local variations in the sum of exchange couplings that connect a given site to other sites

of the system, leading to local variations of the two-sublattice site magnetizations and, as a consequence, one may have local magnetizations that vary in both sign and magnitude. In these identifications, the effective random field at a given site is expressed either in terms of its local magnetization [6], or of the sum of the exchange couplings associated to this site [7].

Since then, many diluted antiferromagnets have been investigated, in such a way that systems like $\text{Fe}_x\text{Zn}_{1-x}\text{F}_2$ and $\text{Fe}_x\text{Mg}_{1-x}\text{Cl}_2$, for certain ranges of concentration x (essentially high values of x , as mentioned above) are nowadays considered as standard experimental realizations of the RFIM [8]. These systems are characterized by large crystal-field anisotropies, so that they may be reasonably well-described in terms of Ising variables. In particular, the compound $\text{Fe}_x\text{Mg}_{1-x}\text{Cl}_2$ behaves like an Ising spin glass for $x < 0.55$, and is considered as a typical RFIM for higher magnetic concentrations. In the RFIM regime, it presents a very curious behavior; one finds a first-order transition turning into a continuous one due to a change in the random fields [8–10]. The concentration at which the first-order transition disappears is estimated to be $x = 0.6$.

From the theoretical point of view, many important questions remain open. At the mean-field level, it is well known that different probability distributions for the random fields may lead to distinct phase diagrams, e.g. a Gaussian probability distribution yields a continuous ferromagnetic–paramagnetic boundary [11], whereas for a bimodal distribution, this boundary exhibits a continuous piece

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at high temperatures ending up at a tricritical point, followed by a first-order phase transition at low temperatures [12]. Indeed, it was argued that whenever an analytic symmetric distribution for the fields presents a minimum at zero field, one should expect a tricritical point and a first-order transition for sufficiently low temperatures [12]; such an argument has been considered further and improved by other authors [13, 14]. The presence of such a first-order transition for sufficiently low temperatures in short-range-interaction models, represents a point that has not been fully elucidated. For the three-dimensional RFIM, high-temperature series expansions [15] and a zero-temperature scaling analysis [16] find continuous transitions for both Gaussian and bimodal distributions. Nevertheless, several zero-temperature studies of the Gaussian three-dimensional RFIM [17–19] suggest a first-order transition for such a model; this occurs because the magnetization and specific-heat critical exponents are very small, and so it is difficult to determine whether the magnetization vanishes continuously, or discontinuously, at the transition. However, in four dimensions a zero-temperature analysis [16] leads to a first-order transition in the bimodal case and a continuous one for a Gaussian distribution, in agreement with the mean-field predictions.

The crossover from first-order to continuous phase transitions has been investigated through different theoretical approaches [10, 20–22]. By means of equilibrium calculations, one possible mechanism used to find such a crossover, or even to suppress the first-order transition completely, consists in introducing an additional kind of randomness in the system, e.g. bond randomness [20, 21]. By considering randomness in the field only, this crossover has been also analyzed through zero-temperature studies, either within a dynamic analysis of abrupt magnetization avalanches and hysteresis phenomena [22], or numerical simulations on a three-dimensional lattice [10, 22]. Since the effects observed in the diluted antiferromagnet $\text{Fe}_x\text{Mg}_{1-x}\text{Cl}_2$ occur for rather low temperatures (typically around 4 K), they may be described satisfactorily by zero-temperature approaches. However, such zero-temperature approaches would not be appropriate for explaining similar effects at higher temperatures, which may possibly be found on similar systems.

In the present work we consider a RFIM that is able to exhibit a critical frontier separating the paramagnetic and ferromagnetic phases, which is qualitatively similar to the one found in [12], i.e. characterized by a tricritical point where a high-temperature continuous critical frontier meets a low-temperature first-order line. In addition to that, by changing the random fields, our model is capable of presenting modifications in the corresponding phase diagram that are not possible within the model of [12]: (i) to change the location of the critical frontier, i.e. to vary the size of the ferromagnetic phase; (ii) to shift the position of the tricritical point, in such a way that the first-order phase transition may be destroyed completely, similarly to what happens in the compound $\text{Fe}_x\text{Mg}_{1-x}\text{Cl}_2$. In such a model, the interactions among spins are of infinite range, i.e. in the limit where the mean-field approach is exact, and the random fields follow a double Gaussian probability distribution, which consists of

a superposition of two Gaussian distributions presenting the same width σ . This distribution recovers in certain limits the simple Gaussian and bimodal probability distributions. We find, analytically a threshold value for σ associated with the destruction of the first-order phase transition line. In the next section we present the model, then find its free energy and phase diagrams. In section 3 we present our conclusions.

2. The model and its solution

Let us define the infinite-range-interaction Ising model in the presence of an external random magnetic field, in terms of the Hamiltonian

$$\mathcal{H} = -\frac{J}{N} \sum_{(i,j)} S_i S_j - \sum_i H_i S_i, \quad (1)$$

where $S_i = \pm 1$ ($i = 1, 2, \dots, N$) and the sum $\sum_{(i,j)}$ applies to all distinct pairs of spins. The random fields $\{H_i\}$ are quenched variables, following a double Gaussian probability distribution,

$$P(H_i) = \frac{1}{2} \left(\frac{1}{2\pi\sigma^2} \right)^{1/2} \left\{ \exp \left[-\frac{(H_i - H_0)^2}{2\sigma^2} \right] + \exp \left[-\frac{(H_i + H_0)^2}{2\sigma^2} \right] \right\}. \quad (2)$$

The probability distribution above depends on two parameters, H_0 and σ , and modifies its form according to the ratio H_0/σ , as exhibited in figure 1. Such a distribution is double-peaked for $(H_0/\sigma) > 1$, presents a single peak for $(H_0/\sigma) < 1$, and changes its concavity at the origin when $(H_0/\sigma) = 1$. Besides that, in the limits $H_0 \rightarrow 0$ and $\sigma \rightarrow 0$, one recovers the symmetric Gaussian and bimodal probability distributions, respectively. Changes between these two limits may be followed by analyzing the moments $\langle H_i^n \rangle_H$ ($n = 1, 2, 3, \dots$) and, in particular, through the kurtosis, $\kappa = \langle H_i^4 \rangle_H / [3(\langle H_i^2 \rangle_H)^2]$, which varies from $\kappa = 1/3$ (bimodal limit) up to $\kappa = 1$ (Gaussian limit), approaching unity in the limit $(H_0/\sigma) \rightarrow 0$, in which case one gets a perfect Gaussian distribution. For finite values of H_0/σ one gets $1/3 < \kappa < 1$, and in particular for the cases exhibited in figure 1, one has that $\kappa \approx 0.97$ [$(H_0/\sigma) = 1/2$], $\kappa \approx 0.83$ [$(H_0/\sigma) = 1$], $\kappa \approx 0.68$ [$(H_0/\sigma) = 3/2$], and $\kappa \approx 0.34$ [$(H_0/\sigma) = 15$].

For a given realization of the site fields $\{H_i\}$, one has a corresponding free energy $F(\{H_i\})$, in such a way that the average over disorder, $[F(\{H_i\})]_H$, becomes

$$[F(\{H_i\})]_H = \int \prod_i [dH_i P(H_i)] F(\{H_i\}). \quad (3)$$

One can now make use of the replica method [23, 24] in order to get the free energy per spin as

$$\begin{aligned} -\beta f &= \lim_{N \rightarrow \infty} \frac{1}{N} [\ln Z(\{H_i\})]_H \\ &= \lim_{N \rightarrow \infty} \lim_{n \rightarrow 0} \frac{1}{Nn} ([Z^n]_H - 1), \end{aligned} \quad (4)$$

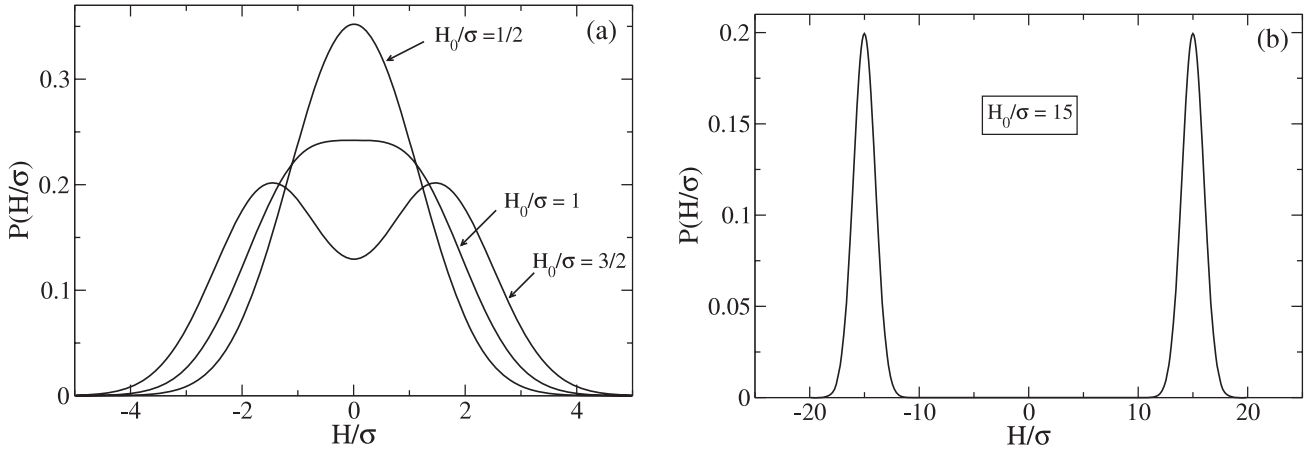


Figure 1. The probability distribution of equation (2) for typical values of the ratio H_0/σ : (a) $(H_0/\sigma) = 1/2, 1, 3/2$; (b) $(H_0/\sigma) = 15$.

where Z^n is the partition function of n copies of the original system defined in equation (1) and $\beta = 1/(kT)$. Standard calculations lead to

$$\beta f = \lim_{n \rightarrow 0} \frac{1}{n} \min g(m^\alpha), \quad (5)$$

where

$$g(m^\alpha) = \frac{\beta J}{2} \sum_{\alpha} (m^\alpha)^2 - \frac{1}{2} \ln \text{Tr}_{\alpha} \exp(\mathcal{H}_{\text{eff}}^+) - \frac{1}{2} \ln \text{Tr}_{\alpha} \exp(\mathcal{H}_{\text{eff}}^-), \quad (6)$$

$$\mathcal{H}_{\text{eff}}^{\pm} = \beta J \sum_{\alpha} m^{\alpha} S^{\alpha} + \beta \sigma \left(\sum_{\alpha} S^{\alpha} \right)^2 \pm \beta H_0 \sum_{\alpha} S^{\alpha}. \quad (7)$$

In the equations above, the index α ($\alpha = 1, 2, \dots, n$) is a replica label and Tr_{α} represents a trace over the spin variables of each replica. The extrema of the functional $g(m^\alpha)$ yields the equilibrium equation for the magnetization of replica α ,

$$m^{\alpha} = \frac{1}{2} \langle S^{\alpha} \rangle_{+} + \frac{1}{2} \langle S^{\alpha} \rangle_{-}, \quad (8)$$

where $\langle \rangle_{\pm}$ refer to thermal averages with respect to the ‘effective Hamiltonians’ $\mathcal{H}_{\text{eff}}^{\pm}$ in equation (7).

If one assumes the replica-symmetry ansatz [23, 24], i.e. $m^{\alpha} = m$ ($\forall \alpha$), the free energy per spin (cf equations (5)–(7)) and the equilibrium condition, equation (8), become

$$f = \frac{J}{2} m^2 - \frac{1}{2\beta} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dz e^{-z^2/2} \ln 2 \cosh \Phi^{+} - \frac{1}{2\beta} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dz e^{-z^2/2} \ln 2 \cosh \Phi^{-}, \quad (9)$$

$$m = \frac{1}{2} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dz e^{-z^2/2} \tanh \Phi^{+} + \frac{1}{2} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dz e^{-z^2/2} \tanh \Phi^{-}, \quad (10)$$

where $\Phi^{\pm} = \beta(Jm + \sigma z \pm H_0)$.

It is important to mention that the present system exhibits no instability associated with the replica symmetric solution [25], which usually appears due to parameters characterized by two replica indices, as in the spin-glass

problem [23, 24]. In the RFIM, one has a single phase transition associated with the magnetization and two phases are possible, namely, the ferromagnetic ($m \neq 0$) and the paramagnetic ($m = 0$) ones. The critical frontier separating these two phases may be found by solving equation (10); in the case of first-order phase transitions, we shall make use of the free energy per spin, equation (9), as well. Let us then expand equation (10) in powers of m ,

$$m = Am + Bm^3 + Cm^5 + O(m^7), \quad (11)$$

where the coefficients are given by

$$A = \beta J \{1 - \rho_1\}, \quad (12)$$

$$B = -\frac{(\beta J)^3}{3} \{1 - 4\rho_1 + 3\rho_2\}, \quad (13)$$

$$C = \frac{(\beta J)^5}{15} \{2 - 17\rho_1 + 30\rho_2 - 15\rho_3\}, \quad (14)$$

with

$$\rho_k = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dz e^{-z^2/2} \tanh^{2k} \beta(H_0 + \sigma z). \quad (15)$$

The continuous critical frontier is determined by setting $A = 1$, provided that $B < 0$. If a first-order critical frontier also occurs, the continuous line ends when $B = 0$; in such cases, the continuous and first-order critical frontiers meet at a tricritical point, whose coordinates may be obtained by solving the equations $A = 1$ and $B = 0$ numerically. In addition to that, for $B > 0$, the first-order critical frontier may be found by equating the free energies at each side of this line, i.e. $f(m = 0) = f(m \neq 0)$.

Using this procedure, we have calculated numerically the critical frontiers separating the paramagnetic and ferromagnetic phases for typical values of σ/J (see figure 2). As will be seen below, the existence of a tricritical point at finite temperatures is restricted to the condition $0 \leq (\sigma/J) \leq \sqrt{2/e\pi}$. At the threshold value $(\sigma/J) = \sqrt{2/e\pi} \cong 0.4839$ the tricritical point occurs at zero temperature.

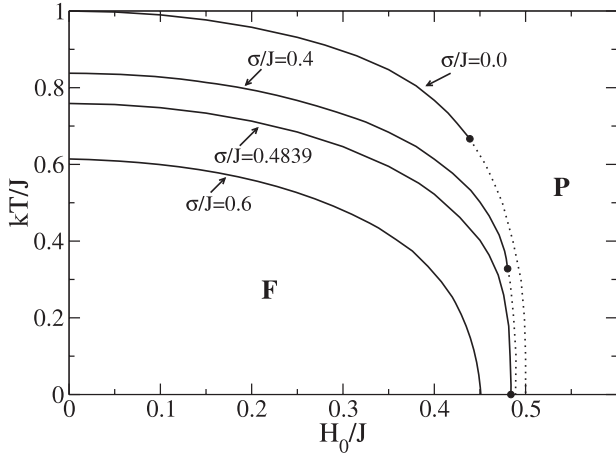


Figure 2. Critical frontiers separating the paramagnetic (**P**) and ferromagnetic (**F**) phases of the infinite-range-interaction ferromagnet in the presence of a double Gaussian random field, for typical values of σ/J . Full (dashed) lines represent continuous (first-order) phase transitions; the black circles are tricritical points. Notice the collapse of the tricritical point at the zero-temperature axis for $(\sigma/J) = 0.4839$.

Let us now analyze how the above-mentioned critical frontier evolves along the zero-temperature axis. At $T = 0$, the free energy and magnetization become, respectively,

$$f = -\frac{J}{2}m^2 - \frac{H_0}{2} \left[\operatorname{erf} \left(\frac{Jm + H_0}{\sigma\sqrt{2}} \right) - \operatorname{erf} \left(\frac{Jm - H_0}{\sigma\sqrt{2}} \right) \right] - \frac{\sigma}{\sqrt{2\pi}} \left\{ \exp \left[-\frac{(Jm + H_0)^2}{2\sigma^2} \right] + \exp \left[-\frac{(Jm - H_0)^2}{2\sigma^2} \right] \right\}, \quad (16)$$

$$m = \frac{1}{2} \operatorname{erf} \left(\frac{Jm + H_0}{\sigma\sqrt{2}} \right) + \frac{1}{2} \operatorname{erf} \left(\frac{Jm - H_0}{\sigma\sqrt{2}} \right). \quad (17)$$

A procedure similar to the one described above for finite temperatures applies in this case, in such a way that one may expand equation (17) in powers of m ,

$$m = am + bm^3 + cm^5 + O(m^7), \quad (18)$$

where

$$a = \sqrt{\frac{2}{\pi}} \left(\frac{J}{\sigma} \right) \exp \left(-\frac{H_0^2}{2\sigma^2} \right), \quad (19)$$

$$b = \frac{1}{6} \sqrt{\frac{2}{\pi}} \left(\frac{J}{\sigma} \right)^3 \left\{ \left(\frac{H_0}{\sigma} \right)^2 - 1 \right\} \exp \left(-\frac{H_0^2}{2\sigma^2} \right), \quad (20)$$

$$c = \frac{1}{120} \sqrt{\frac{2}{\pi}} \left(\frac{J}{\sigma} \right)^5 \left\{ \left(\frac{H_0}{\sigma} \right)^4 - 6 \left(\frac{H_0}{\sigma} \right)^2 + 3 \right\} \times \exp \left(-\frac{H_0^2}{2\sigma^2} \right). \quad (21)$$

A continuous critical frontier occurs at zero temperature for $b < 0$ [i.e. $(H_0/\sigma) < 1$], in such a way that the condition $a = 1$ yields a relation involving H_0/J and σ/J for this critical

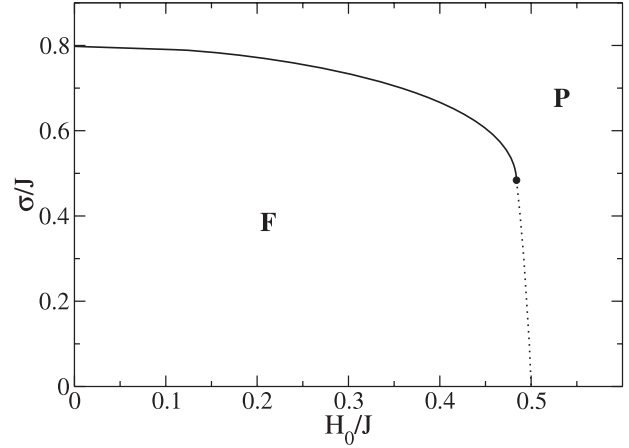


Figure 3. Phase diagram of the infinite-range-interaction ferromagnet in the presence of a double Gaussian random field at zero temperature. The full (dashed) line represents a continuous (first-order) phase transition; the black circle denotes a tricritical point.

frontier,

$$\frac{\sigma}{J} = \sqrt{\frac{2}{\pi}} \exp \left[-\frac{1}{2} \left(\frac{H_0}{J} \right)^2 \left(\frac{J}{\sigma} \right)^2 \right]. \quad (22)$$

One notices that the zero-temperature value of H_0/J decreases, for increasing values of σ/J and, in particular, when $(\sigma/J) = \sqrt{2/\pi}$, one gets $H_0/J = 0$ as a solution. The critical frontier presents a tricritical point at zero temperature given by $b = 0$, $a = 1$,

$$\frac{H_0}{\sigma} = 1, \quad \frac{\sigma}{J} = \sqrt{\frac{2}{e\pi}} \cong 0.4839. \quad (23)$$

This represents the threshold value of σ for the existence of a tricritical point; above this value one gets that $(H_0/\sigma) < 1$, in such a way that the probability distribution of equation (2) presents a single maximum at the origin (cf. figure 1) and there is no tricritical point, i.e. the critical frontier is completely continuous, in agreement with previous analyses [12–14].

For $b > 0$, one gets a first-order critical frontier at zero temperature, which is associated with a tricritical point at finite temperatures. The phase diagram of the model, at zero temperature, is presented in figure 3. Similarly to what happened in the finite-temperature phase diagram, the first-order critical frontier changes into a continuous one, for increasing values of σ/J , just like in other zero-temperature studies of the RFIM [10, 22].

3. Conclusions

Summarizing, the main effects produced by an increase of σ/J in the present model are: (i) a decrease in the extension of the ferromagnetic phase; (ii) in the range of σ/J for which there is a first-order transition line, one observes also a decrease in the extension of such a line; (iii) for sufficiently large values of σ/J , the first-order transitions are transformed into continuous ones. At the threshold value $(\sigma/J) = \sqrt{2/e\pi} \cong 0.4839$,

the tricritical point where the continuous and the first-order transition lines meet, occurs at zero temperature, and for greater values of σ/J , the critical frontier is completely continuous, i.e. there is no tricritical point. Therefore, the ratio σ/J is directly related to the disorder in a real system; for the case of a diluted antiferromagnet, an increase in σ/J should play a similar role to an increase in the dilution.

A crossover of the phase transition from first-order to continuous, due to an increase in the amount of disorder, has been observed in the diluted antiferromagnet $\text{Fe}_x\text{Mg}_{1-x}\text{Cl}_2$, with $0.7 < x < 1.0$ [9, 10]. Such an effect, which has been observed in low—but finite temperatures—has been explained in terms of zero-temperature analyses of different formulations of the RFIM, either through numerical simulations on a three-dimensional lattice [10, 22], or by means of a dynamic study of hysteresis and magnetization avalanches [22]. We believe that the present model is more appropriate for a theoretical description of this effect. In this case, an increase in the measure of randomness in our model, σ/J , would be related to a decrease in the magnetic concentration x , in such a way that the threshold value $(\sigma/J) = \sqrt{2/e\pi}$ would correspond to the critical value $x = 0.6$, at which the first-order transition disappears. In addition to that, the present model may also explain similar effects that could possibly be found, at higher temperatures, on other diluted antiferromagnets.

Finally, we argue that the double Gaussian probability distribution, defined above is suitable for an appropriate theoretical description of the RFIM, being a better candidate for such a purpose than the two most commonly used distributions in the literature.

- (i) In the identifications of the RFIM with diluted antiferromagnets in the presence of a uniform magnetic field, the local random fields are expressed in terms of quantities that vary in both sign and magnitude [6, 7]. This characteristic rules out the bimodal probability distribution from such a class of physical systems.
- (ii) Although the RFIM defined in terms of a simple Gaussian probability distribution for the fields is physically acceptable, it usually leads to a continuous phase transition at finite temperatures, either within mean-field [12–14], or standard short-range-interaction approaches [15, 16]. Such a system is not able to exhibit first-order phase transitions and tricritical points, that may occur in some diluted antiferromagnets [8].
- (iii) By varying appropriately the ratio H_0/σ (a ratio related to the external applied uniform field and the dilution in a real system) in the double Gaussian probability distribution of the present RFIM, one may adjust the model to given physical situations in order to reproduce a wide variety

of physical effects that occur in diluted antiferromagnets, such as continuous and first-order phase transitions, as well as tricritical points.

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