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Phase Transitions

A Multinational Journal

ISSN: (Print) (Online) Journal homepage: https://www.tandfonline.com/loi/gpht20

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PHASE TRANSITIONS
https://doi.org/10.1080/01411594.2022.2162897

Phase diagram of the square 2D Ising lattice with nearest neighbor and next-nearest neighbor interactions

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Abstract

We have determined the temperature dependent phase diagram of the square 2D Ising lattice with anisotropic nearest neighbor ($J_{x,y}$) and isotropic next-nearest neighbor (J_d) interactions. The phase boundaries between the various ordered phases (ferromagnetic, antiferromagnetic and striped antiferromagnetic) and the disordered phase (paramagnetic) are obtained by considering the domain wall free energy. Although the phase boundary equations are not exact, they provide a very accurate description when the nearest neighbor interactions are stronger than the next-nearest neighbor interaction. The square 2D Ising lattice does not exhibit a phase transition when $J_d = -\frac{1}{2}|J_{x,y}|_{\min}$ if J_x and J_y have the same sign or $J_d = \frac{1}{2}|J_{x,y}|_{\min}$ if J_x and J_y have opposite signs.

ARTICLE HISTORY
Received 1 September 2022
Accepted 21 December 2022

KEYWORDS
Phase diagram; Ising; domain wall free energy; order–disorder phase transition

Introduction

In Nature one often encounters phase transitions, i.e. transformations of a material from one state to another state. For example at 0°C and under atmospheric conditions water undergoes a transition from its liquid state to its solid state (ice). Despite the omnipresence of phase transitions in real life, mathematical descriptions of phase transitions are often lacking because of their complexity. In fact there are only a handful of phase transitions that have been exactly solved using statistical mechanical methods [1]. One of the most simplest models is the so-called Ising model. In 1925 Ernst Ising proposed a simple model to describe ferromagnetism [2]. He considered a one-dimensional chain of spins. The spin, s, can only take two values, $s = +1$ or $s = -1$, where $s = +1$ refers to the spin pointing upwards and $s = -1$ refers to the spin pointing downwards. The spins only interact with their nearest neighbors via a coupling constant J. Neighboring spins prefer to align in the ferromagnetic (or antiferromagnetic) configuration if $J > 0$ (or $J < 0$). Ising found that the spin chain is only ordered at $T = 0\ K$ and disordered at any nonzero temperature. This result is easy to understand if one considers the free energy, $F = E - TS$, that is required to flip a single spin somewhere in the infinite long chain. The free energy, F, that is required to flip a single spin is $2J - kTln(N)$. Irrespective of the actual strength of the interaction between neighboring spins, the entropy term will always dominate as $N \to \infty$ (provided at least that $T > 0\ K$) and therefore the free energy for a spin flip is always negative.

Based on his findings for the one-dimensional (1D) system, Ising conjectured that also the two-dimensional (2D) and three-dimensional (3D) Ising systems have a critical temperature of $0\ K$. In

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1936 Peierls [3] demonstrated, however, that the conjecture of Ising is not correct. The 2D and 3D Ising systems have a nonzero phase transition temperature. Below the critical temperature, these systems are in an ordered state (e.g. ferromagnetic or antiferromagnetic), whereas above the critical temperature these systems are in a disordered (paramagnetic) state.

After Ising solved the 1D Ising model it took almost two decades before the square 2D Ising model was solved by Lars Onsager [4]. Several years before Onsager published his seminal article, Kramers and Wannier [5] already demonstrated that if the 2D Ising model with ferromagnetic isotropic nearest neighbor interactions has an order–disorder phase transition, the transition temperature is uniquely defined by the relation $\sinh(2J/k_bT_c) = 1$. In 1944 Onsager showed that the 2D Ising model indeed exhibits an order–disorder phase transition. Onsager derived an exact expression for the free energy per spin in the absence of an external magnetic field. Unfortunately, the free energy per spin does not give a full understanding of all the properties of the system. There are many interesting quantities such as the spontaneous magnetization, susceptibilities and correlation functions, that cannot be directly deduced from the free energy per spin. Despite the long history of Ising systems they still receive substantial attention [6–9]. To date more complicated 2D Ising lattices that involve interactions beyond nearest neighbor interactions or an external field have not yet been solved exactly.

After the publication of the exaction solution of the square 2D Ising model with nearest neighbor interactions by Onsager in 1944 more than 1500 papers have been appeared in the literature that have either two-dimensional Ising or 2D Ising in their title. Particularly in the last few decades several theoretical papers have been published on the 2D Ising model with interactions that go beyond the nearest-neighbor interactions. Several of these papers [10,11] make use of the domain wall method that has been put forward in 2006 [12], while others elaborate on parts of the phase diagram [13,14], partition function zeros [15] or critical properties of the antiferromagnetic 2D Ising system with nearest and next-nearest neighbor interactions [16]. More recently, Gagliardi and Pierre-Louis [17] used the results of 2D Ising model with nearest and next-nearest neighbor interactions to study the equilibrium island shape in crystal growth. Despite the fact that several studies deal with the phase diagram of the square 2D Ising lattice with nearest and next-nearest neighbor interactions a complete and accurate phase diagram is still lacking. It is the aim of this work to bridge this gap and provide a complete phase diagram.

The 2D Ising model has been used to describe and interpret a large number of surface processes, such order–disorder phase transitions [18], step diffusivity [19] and domain wall wandering [20,21]. In the vast majority of cases these systems are compared to the 2D Ising model with only nearest neighbor interactions. The experimental systems are, however, usually more realistically modelled by a 2D Ising model that also involves next-nearest neighbor interactions. These next-nearest neighbor interactions are virtually in all cases weaker than the nearest-neighbor interactions. The latter is very fortunate as the results obtained by our analysis are most accurate in the range where the next-nearest neighbor interactions are weaker than the nearest neighbor interactions.

Here we will consider a square 2D Ising lattice with anisotropic nearest neighbor and isotropic next-nearest neighbor interactions. We will derive the full phase diagram by using a method that relies on the determination of the free energy of domain walls between two regions with opposite spin order. The critical temperature is found by setting the domain wall free energy equal to zero. This method is, unfortunately, not exact, but it provides very accurate results if the nearest-neighbor interactions are not too weak. Furthermore, we show that under certain conditions the square 2D Ising lattice with nearest neighbor and next-nearest neighbor interactions does not exhibit a phase transition.

Results and discussion

Let us consider a two-dimensional square lattice with anisotropic nearest neighbor ($J_{x,y}$) and isotropic next-nearest neighbor (J_d) interactions. $J > 0$ and $J < 0$ refer to ferromagnetic and antiferromagnetic interactions, respectively. The Hamiltonian of this system is given by,

$$H = -J_x \sum_i s_{i,j}s_{i+1,j} - J_y \sum_j s_{i,j}s_{i,j+1} - J_d \sum_{i,j} (s_{i,j}s_{i+1,\,j+1} + s_{i,j}s_{i+1,j-1}) \tag{1}$$

We will first consider the 2D Ising square lattice with ferromagnetic nearest neighbor interactions, see Figure 1. The dotted line refers to a domain boundary running along the x-direction (we will refer to this direction as the (10) direction). This boundary separates two regions with opposite spin orientation. The formation energy per unit length of a (10) domain boundary is $2J_y + 4J_d$, whereas the formation energy of a kink with a length of n units is given by [12],

$$E_{kink,\,n} = 2nJ_x + 4(n-1)J_d \tag{2}$$

The Ising lattice is ordered at $T = 0\,K$ if the domain wall formation energies (in any direction) are all positive. As the (10) and (01) domain boundaries have the lowest formation energies we find that this system is in its ferromagnetic phase if,

$$J_d > -\frac{1}{2}(J_{x,y})_{\min} \tag{3}$$

We can extend this analysis to the antiferromagnetic and striped antiferromagnetic phases. The results are summarized in Table 1 and the $T = 0\,K$ phase diagram of the 2D Ising lattice with nearest and next-nearest neighbor interactions is shown in Figure 2.

In the case of ferromagnetic or antiferromagnetic nearest neighbor interactions the ground state switches from the (anti)ferromagnetic phase to one of the striped antiferromagnetic phases when

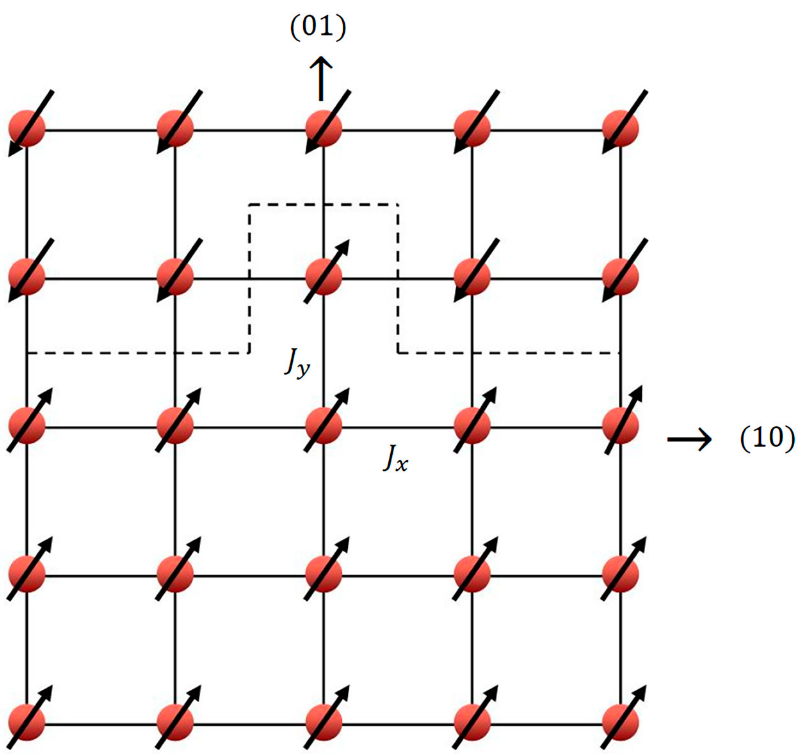

Figure 1. Schematic diagram of the square 2D Ising lattice with anisotropic ferromagnetic nearest neighbor ($J_{x,y}$) and isotropic next-nearest neighbor (J_d) interactions The dotted line is a domain boundary running in the (10) direction that separates two regions with opposite spin orientations.

Table 1. Energy per spin and domain wall formation energies for (10) and (10) directions of the (anti)ferromagnetic and striped antiferromagnetic ground states.

Phase	Energy per spin	$E_{(10)}$	$E_{(01)}$
F + + + + + + + + +	$-2J_x - 2J_y - 4J_d$ $J_x + J_y > 0$	$2J_y + 4J_d$ $J_y + 2J_d > 0$	$2J_x + 4J_d$ $J_x + 2J_d > 0$
AF + - + - + - + - +	$2J_x + 2J_y - 4J_d$ $J_x + J_y < 0$	$-2J_y + 4J_d$ $2J_d - J_y > 0$	$-2J_x + 4J_d$ $2J_d - J_x > 0$
SAF1 - - - + + + - - -	$-2J_x + 2J_y + 4J_d$ $J_x - J_y > 0$	$-2J_y - 4J_d$ $2J_d + J_y < 0$	$2J_x - 4J_d$ $J_x - 2J_d > 0$
SAF2 - + - - + - - + -	$2J_x - 2J_y + 4J_d$ $J_x - J_y < 0$	$2J_y - 4J_d$ $J_y - 2J_d > 0$	$-2J_x - 4J_d$ $2J_d + J_x < 0$

$J_d < -\frac{1}{2}|J_{x,y}|_{\min}$ (see Figure 2(a)). In the case that one nearest neighbor interaction is ferromagnetic and the other one antiferromagnetic, the striped antiferromagnetic phase switches to the ferromagnetic or antiferromagnetic phase when $J_d > \frac{1}{2}|J_{x,y}|_{\min}$ (see Figure 2(b)). The domain wall formation energy of one of the (01)/(10) boundaries is always zero when $J_d = -\frac{1}{2}|J_{x,y}|_{\min}$ if J_x and J_y have the same sign or $J_d = \frac{1}{2}|J_{x,y}|_{\min}$ if J_x and J_y have opposite signs. The latter implies that in these cases the square 2D Ising lattice is in its paramagnetic phase at $T = 0$ K and therefore the system does *not* exhibit a phase transition. It is important to mention here that the other two phase boundaries

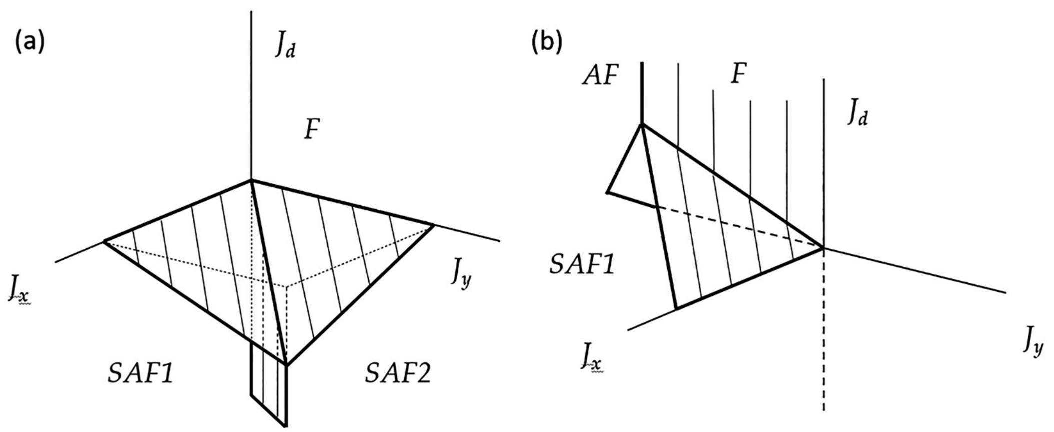

Figure 2. Two quadrants of the phase diagram of the square 2D Ising lattice with anisotropic nearest neighbor and isotropic next-nearest neighbor interactions at T = 0 K. (a) Both nearest-neighbor interactions have the same sign ($J_{x,y} > 0$ or $J_{x,y} < 0$). (b) The nearest-neighbor interactions have opposite signs ($J_x > 0$ and $J_y < 0$ or $J_x < 0$ and $J_y > 0$). F, AF and SAF1 and SAF2 refer to ferromagnetic, antiferromagnetic and the two striped antiferromagnetic phases, respectively.

between the ferromagnetic/antiferromagnetic phases and the two striped antiferromagnetic phases, respectively, are different in the sense that the domain wall formation energies (in any direction) are always positive and therefore these transitions are regular first-order transitions.

We now return to the ferromagnetic system and discuss how the system behaves at nonzero temperatures. With increasing temperature, the number of kinks in the domain wall increases. These kinks costs energy, but will also lead to an increase of the entropy. As the entropy term increases with increasing temperature there is a temperature at which the entropy term outweighs the kink formation energy term. At this temperature, T_c, the domain wall free energy vanishes and the system undergoes a phase transition from the ordered phase to the disorder phase.

In order to find this critical temperature we need the partition sum of the domain boundary. The partition sum of a (10) domain wall is given by [12],

$$Z_{(10)} = \sum_i e^{-E_i/k_bT} = e^{-(2J_y+4J_d)/k_bT}\left(1 + 2\sum_{n=1}^{\infty} e^{-(2nJ_x+4(n-1)J_d)/k_bT}\right) \tag{4}$$

The free energy of the (10) domain wall per unit length is,

$$F_{(10)} = -k_bTln(Z_{(10)}) = 2J_y + 4J_d - k_bTln\left(1 + \frac{2e^{-2J_x/k_bT}}{1 - e^{-2(J_x+2J_d)/k_bT}}\right) \tag{5}$$

The critical temperature can be found by setting the domain wall free energy equal to zero. We find,

$$e^{-2J_x/k_bT_c} + e^{-2J_y/k_bT_c} + e^{-2(J_x+J_y)/k_bT_c}(2 - e^{-4J_d/k_bT_c}) = e^{4J_d/k_bT_c} \tag{6}$$

We can extend this analysis to the antiferromagnetic case by simply replacing J_x and J_y by $-J_x$ and $-J_y$. The formation energy per unit length of a (10) domain boundary is then $-2J_y + 4J_d$ and the formation energy of kink with a length of n units is given by $E_{kink,\,n} = -2nJ_x + 4(n-1)J_d$. By following the same route as outlined above we find that the critical temperature is given by,

$$e^{2J_x/k_bT_c} + e^{2J_y/k_bT_c} + e^{2(J_x+J_y)/k_bT_c}(2 - e^{-4J_d/k_bT_c}) = e^{4J_d/k_bT_c} \tag{7}$$

This expression is identical to Equation (6) apart from the change in sign of J_x and J_y. For the sake of simplicity we first elaborate on the phase diagram of the 2D Ising lattice with isotropic nearest neighbor and next-nearest neighbor interactions. By solving Equations (6) and (7) we find,

$$J_d/k_bT_c = -\frac{1}{4}ln\left[\frac{(2 + e^{-2|J_x|/k_bT_c}) \pm \sqrt{e^{-4|J_x|/k_bT_c} + 4e^{-2|J_x|/k_bT_c}}}{2e^{-2|J_x|/k_bT_c}}\right] \tag{8}$$

Please note that the + solution has to be ignored as for this value of J_d the ground state of the system is not the ferromagnetic or antiferromagnetic phase.

So far, we have assumed that both nearest neighbor interactions are either ferromagnetic or antiferromagnetic. However, with a few minor modifications Equation (6) can also be applied to the striped antiferromagnetic systems. For the phase boundaries between the striped antiferromagnetic phases and the paramagnetic phase J_y and J_d have to be replaced by by $-J_y$ and $-J_d$, respectively, if $J_y > J_x$ (or J_x by $-J_x$ and J_d by $-J_d$ if $J_y < J_x$). For the striped antiferromagnetic phases we find an asymptote when $J_d = \frac{1}{2}|J_{x,y}|_{\text{min}}$. In Table 2 an overview of the phase boundary equations is given.

As our model is not exact, it is appropriate to elaborate on the applicability range of our results. In Figure 3 we show several cross sections of the phase diagram. In Figure 3(a) the nearest neighbor interaction is isotropic ($J_y = J_x$). The agreement between Equation (6) and the available numerical results is very good [22–26] (the critical temperature deviates less than 1% from the available numerical data when $J_d < \frac{1}{3}J_x$). For a vanishing next-nearest neighbor interaction energy the exact result of Onsager [4] is recovered. In the vicinity of the Onsager point, i.e.

Table 2. Phase boundary equations for the ferromagnetic, antiferromagnetic and striped antiferromagnetic phases.

Phase	J_x, J_y, J_d	Phase boundary equation
F		
+ + +	$J_x + J_y > 0$	$e^{-2J_x/k_bT_c} + e^{-2J_y/k_bT_c} + e^{-2(J_x+J_y)/k_bT_c}(2 - e^{-4J_d/k_bT_c}) = e^{4J_d/k_bT_c}$
+ + +	$J_y + 2J_d > 0$	
+ + +	$J_x + 2J_d > 0$	
AF		
+ - +	$J_x + J_y < 0$	$e^{2J_x/k_bT_c} + e^{2J_y/k_bT_c} + e^{2(J_x+J_y)/k_bT_c}(2 - e^{-4J_d/k_bT_c}) = e^{4J_d/k_bT_c}$
- + -	$2J_d - J_y > 0$	
+ - +	$2J_d - J_x > 0$	
SAF1		
- - -	$J_x - J_y > 0$	$e^{-2J_x/k_bT_c} + e^{2J_y/k_bT_c} + e^{-2(J_x-J_y)/k_bT_c}(2 - e^{4J_d/k_bT_c}) = e^{-4J_d/k_bT_c}$
+ + +	$2J_d + J_y < 0$	
- - -	$J_x - 2J_d > 0$	
SAF2		
- + -	$J_x - J_y < 0$	$e^{2J_x/k_bT_c} + e^{-2J_y/k_bT_c} + e^{-2(-J_x+J_y)/k_bT_c}(2 - e^{4J_d/k_bT_c}) = e^{-4J_d/k_bT_c}$
- + -	$J_y - 2J_d > 0$	
- + -	$2J_d + J_x < 0$	

$\frac{J_x}{k_bT_c} = \frac{1}{2}ln\left(\sqrt{2}+1\right)$ and $J_d = 0$ we use Equation (6) to determine the derivative $\left(\frac{dJ_d}{dJ_x}\right)_{J_d=0}$. We find, $\left(\frac{dJ_d}{dJ_x}\right)_{J_d=0} = -\frac{1}{2}\sqrt{2}$ [27]. This result is also exact, as it agrees with the value obtained from spin–spin correlation functions [28]. For a vanishing nearest neighbor interaction energy the results are, however, less accurate. If $J_x = 0$ the square 2D Ising lattice decouples into two interpenetrating square 2D Ising lattices. These two interpenetrating square 2D lattices have an isotropic nearest neighbor interaction J_d, resulting in a critical temperature $\frac{J_d}{k_bT_c} = \frac{1}{2}ln\left(\sqrt{2}+1\right) \approx 0.4406867...$. From Equation (6) we, however, find $cosh\left(\frac{4J_d}{k_bT_c}\right) = 2$, which results in $\frac{J_d}{k_bT_c} = \frac{1}{4}ln\left(\sqrt{3}+2\right) \approx 0.3292394\ldots$ This result is obviously wrong, indicating that our model fails to describe the regime near the decoupling properly [10]. Using renormalization group theory van Leeuwen has shown [29] that the critical temperature in the vicinity of the decoupling regime ($J_x \to 0$) has a cusp and behaves as, $\frac{J_d}{k_bT_c} \propto \left(H_c - \frac{J_x}{k_bT_c}\right)^{4/7}$, where, $H_c = \frac{1}{2}ln\left(\sqrt{2}+1\right)$. For a vanishing nearest neighbor interaction our model also reveals a cusp in the phase boundary between the (anti)ferromagnetic phase and paramagnetic phase.

The fact that in the case of a vanishing next-nearest neighbor interaction the partition function, i.e. Equation (4), is exact for all temperatures implies that we have the correct set of Boltzmann factors. This is remarkable as we have ignored overhangs and inclusions. Apparently the extra terms perfectly cancel. However, when we introduce a next-nearest neighbor interaction the partition function is not exact anymore. The latter is intimately related to the fact that the Boltzmann terms of kinked and non-kinked contributions to the partition function are different for a non-zero next nearest neighbor interaction. A kinked segment costs energy $2J_x + 2J_d$, whereas a non-kinked segment costs energy $2J_x + 4J_d$. In our analysis, see Equation (4), the number of kinked segments per configuration is limited to the absolute minimum of only one and therefore the partition

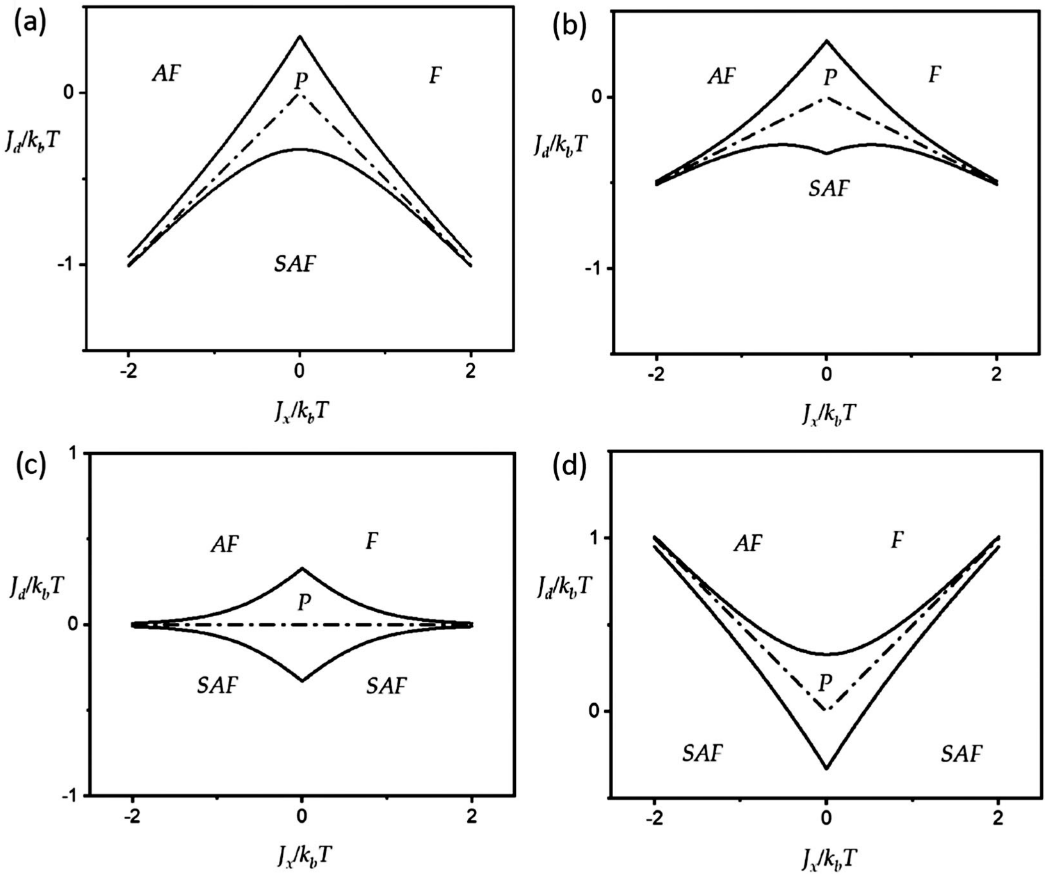

Figure 3. Various cross sections of the phase diagram of the 2D square Ising model with anisotropic nearest neighbor ($J_{x,y}$) and isotropic next-nearest neighbor (J_d) interactions (a) $J_y = J_x$ (b) $J_y = 2J_x$ (c) $J_y = 0$ and (d) $J_y = -J_x$. Please note that: (1) all phase boundaries are invariant under the transformation $J_x \to -J_x$ and (2) the phase boundaries in panels (a) and (d) are mirror symmetric under the transformation $J_d \to -J_d$.

function $Z_{(10)}$ exhibits a maximum for $J_d > 0$ and a minimum for $J_d < 0$, respectively. This implies that for $J_d > 0$ our method gives an upper bound on the critical temperature. Likewise for $J_d < 0$ our method results in a lower bound on the critical temperature.

In Figure 3(b) the nearest neighbor interactions are anisotropic ($J_y = 2J_x$). We observe the development of a cusp in the phase boundary between the striped antiferromagnetic phase and the paramagnetic phase. In Figure 3(c) one of the nearest neighbor interactions is set to zero ($J_y = 0$). Both phase boundaries have a cusp for a vanishing nearest neighbor interaction. In addition, for a vanishing next-nearest neighbor interaction the system converts to a 1D Ising system. This system is disordered at any non-zero temperature and does not exhibit a phase transition.

Finally, in Figure 3(d) we consider the case that the one nearest neighbor interaction is ferromagnetic, while the other nearest neighbor interaction is antiferromagnetic. There is a cusp in the striped antiferromagnetic to paramagnetic phase boundary, while there is no cusp in the (anti)ferromagnetic to striped antiferromagnetic phase boundary.

Conclusions

We have presented the full temperature dependent phase diagram of the square 2D Ising lattice with anisotropic nearest neighbor and isotropic next-nearest neighbor interactions. The phase boundaries between the various ordered phases ((anti)ferromagnetic and striped antiferromagnetic) and the paramagnetic phase are obtained by a statistical mechanics method that relies on the determination of the domain wall free energy between two regions with opposite sign ordering. The square 2D Ising lattice with anisotropic nearest neighbor and isotropic next-nearest neighbor interactions does not exhibit a phase transition for $J_d = -\frac{1}{2}|J_{x,y}|_{\min}$ if J_x and J_y have the same sign or $J_d = \frac{1}{2}|J_{x,y}|_{\min}$ if J_x and J_y have opposite signs.

Disclosure statement

No potential conflict of interest was reported by the author(s).

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