Casimir force within Ising chain with competing interactions

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We derive exact results for the critical Casimir force (CCF) within the one-dimensional Ising model with periodic boundary conditions (PBC's) and long-range equivalent-neighbor ferromagnetic interactions of strength $J_l/N > 0$ superimposed on the nearest-neighbor interactions of strength J_s which could be either ferromagnetic ($J_s > 0$) or antiferromagnetic ($J_s < 0$). In the infinite system limit the model, also known as the Nagle-Kardar model, exhibits in the plane $(K_s = \beta J_s, K_l = \beta J_l)$ a critical line $2K_l = \exp(-2K_s), K_s > -\ln 3/4$, which ends at a tricritical point $(K_l = -\sqrt{3}/2, K_s = -\ln 3/4)$. The critical Casimir amplitudes are: $\Delta_{\rm Cas}^{\rm (cr)} = 1/4$ at the critical line, and $\Delta_{\rm Cas}^{\rm (tr)} = 1/3$ at the tricritical point. Quite unexpectedly, with the imposed PBC's the CCF exhibits very unusual behavior as a function of temperature and magnetic field. It is *repulsive* near the critical line and tricritical point, decaying rapidly with separation from those two singular regimes fast away from them and becoming *attractive*, displaying in which the maximum amplitude of the attraction exceeds the maximum amplitude of repulsion. This represents a violation of the widely-accepted "boundary condition rule," which holds that the CCF is attractive for equivalent BC's and repulsive for conflicting BC's *independently* of the actual bulk universality class of the phase transition under investigation.

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Introduction: We consider the Casimir effect in a model Hamiltonian [1–3] with two competing interactions: the Ising model on a chain with " nearest-neighbor" and with "infinitesimal equivalent-neighbor" interactions between the spins. This is known also as the Nagle-Kardar model (for reviews see [4–6]). The Hamiltonian of the model is:

$$\beta\mathcal{H}_{NK}(K_l,K_s,h) = -K_s\sum_{\langle i,j\rangle}^{N} S_iS_j + h\sum_{i=1}^{N} S_i + \\ -\frac{K_l}{N}\sum_{i,j=1}^{N} S_iS_j, \quad K_s, h \in \mathbb{R}, \quad K_l \in \mathbb{R}^+, \tag{1}$$

where the following notations: $K_s = \beta J_s$, $K_l = \beta J_l$, $h = \beta H$, $\beta = 1/(k_BT)$, $k_B = 1$ are used. Given the symmetry of the problem it suffices to fix $h \geq 0$.

The first two terms on the right hand side of (1) describes the Ising model with short-ranged interactions between nearest neighbors in a magnetic field h, on a spin chain with *periodic boundary conditions* and with $S_i = \pm 1, i = 1, \cdots, N$ with interaction constant J_s. The second term is the equivalent-neighbor Ising model with infinitesimal long-ranged interaction between spins characterized by J_l. The nearest-neighbor interaction is either ferromagnetic or antiferromagnetic, i.e., $K_s > 0$ or $K_s < 0$, while the long-range interaction is always ferromagnetic, i.e., $K_l > 0$. When $K_l < 0$ there is no order at finite temperature.

This model was introduced by Baker in 1969 [1]. The seminal contributions of Nagle [2] and Kardar [3] demonstrated that the model is instructive as a means to analyze complicated phase diagrams and crossover phenomena arising from the competition between ferromagnetic and antiferromagnetic interactions. The range of subsequent work highlights the widespread interest in the properties and implications of the system [4–20], which has proven to be a fertile platform for the investigation of various generalizations of the competition between the antiferromagnetic and ferromagnetic interactions [18, 19, 21–28]. In particular it has been shown that this simple system may well describe a number of interesting phenomena, including ensemble inequivalence [13, 15, 28], negative specific heat[13–15], ergodicity breaking [13–15], long-lived thermodynamically unstable states [13, 14], the prospect of analysis of different information estimators [21] and the cooling process of a long-range system [29].

We have discovered that the behavior of this system is interesting not only in the thermodynamic limit, in which its phase diagram is highly non-trivial, see Fig. 1, but also when the system is finite, in which case the fluctuation-induced critical Casimir force (CCF) exhibits unusually rich structure – see Figs. 2 and 3. Below we briefly explain how we obtained the results shown there.

Finite-size Gibbs free energy density (GFE): In order to determine the behavior of the CCF we need to know the Gibbs free energies in the finite and infinite Ising chains with a given magnetic field h.

The Gibbs free energy per spin is given by

$$f_N[\mathcal{H}_{NK}(K_l,K_s,h)] \equiv f_N(K_s,K_l,h) = \\ -(\beta N)^{-1}\ln Z_N(K_s,K_l,h), \tag{2}$$

where $Z_N(K_s, K_l, h)$ is the grand canonical partition function of the model. Further on, we will omit the arguments K_s, K_l (and h), where this does not lead to misunderstanding.

The partition function for finite N may be obtained by the well-known transfer matrix technique

$$Z_N(K_s, K_l, h) = I_N^p (K_s, K_l, h) + I_N^m (K_s, K_l, h), \quad (3)$$

where

$$I_N^{p,m} (K_s, K_l, h) = \sqrt{\frac{N}{4\pi K_l}} \int_{-\infty}^{\infty} e^{-N\Psi_{p,m}(y)} dy, \quad (4)$$

with

$$\Psi_{p,m}(y) \, (\equiv \Psi_{p,m}(y|K_s, K_l, h)) = \frac{y^2}{4K_l} - \ln \lambda_{p,m}(h + y). \quad (5)$$

Here

$$\lambda_{p,m} = e^{K_s} \cosh(h + y) \pm \sqrt{e^{2K_s} \sinh^2(h + y) + e^{-2K_s}} \quad (6)$$

are the eigenvalues of the corresponding transfer matrix of the one-dimensional Ising model in a field $h + y$.

Since in Eq. (4) $N \gg 1$ we will calculate integrals by the Laplace method. Thus, we are interested in minimum value(s) of functions $\Psi_k(y)$, $k = p, m$. We will see that such minima always exist at some $y_p^{\pm} = y_p^{\pm}(K_s, K_l, h)$ and $y_m^{\pm} = y_m^{\pm}(K_s, K_l, h)$. The subscript $k\,(k = "p" \text{ or } "m")$ indicates if λ_p or λ_m enters the corresponding function $\Psi_k(y)$, while superscript $l\,(l = "+" \text{ or } "-")$ is used to indicate whether the minimum lies in the $[0, \infty]$ or $[-\infty, 0]$ regions of integration. From (5) one finds that $y_k^{\pm} = y_k^{\pm}(K_l, K_s, h)$ satisfy the equations

$$y_k^{\pm} = \pm \frac{2K_l \sinh(h + y_k^{\pm})}{\sqrt{\sinh^2(h + y_k^{\pm}) + e^{-4K_s}}}, \quad k = p, m. \quad (7)$$

We stress that $y_{p,m}^{\pm}$ do *not* depend on N. For $h = 0$ these equations always have as solutions $y_p^{\pm} = y_m^{\pm} = 0$.

As it will become clear later, we are interested in cases in which an expansion of the free energy in terms of the mean magnetization, m, starts a power of m equal to $2n$ with $n \geq 1$. In such cases and for N large, integrals of type (4) can be estimated by the (generalized) Laplace method [30], which states that, if on the finite interval $[a, b] \in \mathbb{R}$ the function $f(x)$ has a single minimum at x_0, such that $a < x_0 < b$, $f^{(j)}(x_0) = 0$ (here (j) means $j-th$ derivative with respect to x) with $1 \leq j \leq 2n - 1$, and $f^{(2n)}(x_0) \neq 0$, with $n \geq 1$, then

$$g(N) = \int_a^b \exp[-Nf(x)]dx \simeq \Gamma\left(\frac{1}{2n}\right) \frac{[2n!]^{1/(2n)}}{n} \times \frac{1}{N^{1/(2n)}} \frac{\exp[-Nf(x_0)]}{\sqrt{f^{(2n)}(x_0)}} \left(1 + \mathcal{O}\left(N^{-1/n}\right)\right). \quad (8)$$

In the case of the existence of a *single* minimum y_k^+ (the choice $h > 0$ implies y_k^+) with respect to y of the functions $\Psi_k(y)$, $k = p, m$ and *where* $\Psi_k^{(11)}(y_{p,m}) > 0$, using the Eq.(8), with $j = n = 1$, for evaluating the integrals in Eq. (3) for $N \gg 1$, we deduce for the GFE the result

$$\beta f_N(K_s, K_l, h) = \Psi_1(y_p^+) + \frac{1}{2N} \ln\left[2K_l \Psi_p^{(11)}(y_p^+)\right] - \frac{1}{N} \ln\left\{1 + \Upsilon(y_p^+, y_m^+) e^{[-N\Phi(y_p^+, y_p^-)]} \left[1 + \mathcal{O}(N^{-1})\right]\right\} \quad (9)$$

where the shorthands

$$\Upsilon(y_p^+, y_m^+) \equiv \sqrt{\frac{\Psi_p^{(11)}(y_p^+)}{\Psi_m^{(11)}(y_m^+)}}, \; \Phi(y_p^+, y_m^+) \equiv \Psi_m(y_m^+) - \Psi_p(y_p^+)$$

are used. We recall that in deriving Eq. (9) we have assumed that $\Psi_p^{(11)}(y_p^+) > 0$ and $\Psi_m^{(11)}(y_m^+) > 0$, with $y_{\pm}$ determined from $\Psi_{p,m}^{(1)}(y_{p,m}) = 0$. When $h \neq 0$ equations (7) have a single solution, i.e., any of the functions $\Psi_{p,m}(y)$ posses a single *global* minimum with respect to y. When $h = 0$ this is *not* the case. As $\lambda_p(y) > \lambda_m(y)$, for al values of y, and so $\Psi_p(y) < \Psi_m(y)$, thus only $\Psi_p(y)$ will determine the *bulk* behavior of the system. Now, there is no difficulty in verifying that GFE in the bulk is defined as

$$\beta f_\infty[\mathcal{H}_{NK}(h)] = \inf_m \left\{\frac{1}{2}m^2 - \ln[\lambda_p(2K_l m)]\right\}. \quad (10)$$

The value of m which minimizes the expression in the curly brackets is the uniform magnetization: $m = \lim_{N\to\infty} \sum_i S_i/N$. Here the fact is used that the value of y at which the function $\Psi_p(y)$ reaches its minimum is proportional to the magnetization per spin, i.e. $y = y_p^+ = 2K_l m$. Eq. (10) has been obtained by Kardar [3].

Phase diagram: The presentation of the Gibbs free energy, Eq.(10), in terms of the power of magnetization has the form [3]

$$f_\infty(K_l, K_s, h = 0) = \inf_m \Big\{ -\ln[2\cosh(K_s)] - K_l \left(2K_l e^{2K_s} - 1\right) m^2 + (2/3) K_l^4 e^{2K_s} \left(3e^{4K_s} - 1\right) m^4 + \mathcal{O}(m^6) \Big\} \quad (11)$$

From here we immediately conclude the existence of a line of critical points $2K_l = \exp(-2K_s), K_s > -\ln 3/4$ (then the multiplier in front of m^2 equals zero, while the one in front of m^4 is positive). If, however, $K_s > -\ln 3/4$ the second term will be also zero and we obtain the condition for the existence of a tricritical point. Its coordinates trivially are $(K_l = -\sqrt{3}/2, K_s = -\ln 3/4)$. The determination of the phase diagram in terms of T given the values of J_s and J_l is, however, not so trivial. It can be achived numerically, as in Refs. [2, 3, 12, 13, 20, 21, 31]. The result, which is well known, is shown in Fig. 1. Here we briefly explain how this phase diagram can be also obtained analytically in terms of the Lambert W-function[32] (also known as omega function or product logarithm; in what follows we use only its principal branch) $W_p(x)$ such that $W_p(x)\exp[W_p(x)] = x$. Using its properties, it is easy to show that, when $x > -1/e$, at the critical line (the red line in Fig. 1) one has $T_c = 2J_s/W_p(x) = J_l[2x/W_p(x)]$, where $x \equiv K_s/K_l = J_s/J_l$. At this line the spontaneous magnetization critical exponent $\beta = 1/2$ [2]. The green point marks the tricritical point C with coordinates $\{y_{\rm TP} = 2\exp[W_p(-\ln(3)/(2\sqrt{3}))] = 2/\sqrt{3}, x_{\rm TP} = -\ln(3)/(2\sqrt{3}) \simeq -0.317\}$. There the spontaneous magnetization critical exponent $\beta = 1/4$. The diagram also shows that a zero field first-order transition temperature (the blue line) meets the second order transition line at point C that ends at $x = -0.5$. At this line three phases with the same free energy and magnetization $m = 0, m = \pm m_{\rm trc}$ coexist. Above this line at zero external field the magnetization is zero, while below it there are two phases with nonzero magnetization. Since $W_p(\infty) \to \infty$ and $W_p(0) = 0$, we have for the critical temperature $T_c(J_s \to 0, J_l) = 2J_l$ and $T_c(J_s, J_l \to 0) = 0$.

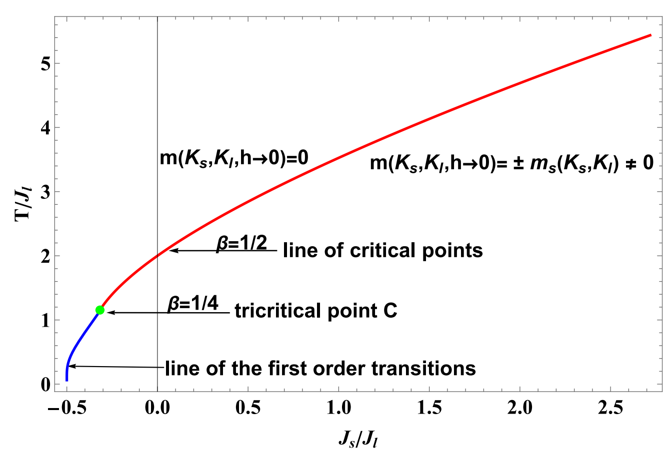

FIG. 1. The phase diagram in terms of the temperature, shown as a function of J_s and J_l. The red line $T/J_l = 2W_p(x)$ represents a line of critical points, while the green point marks the tricritical point C with coordinates $\{y_{\rm TP} = 2/\sqrt{3}, x_{\rm TP} = -\ln(3)/(2\sqrt{3})\}$. A zero field first-order transition temperature (the blue line) meets the second order transition line at point C and ends at $x = -0.5$.

Casimir force (CF): Under the assumption that the finite system of length N is in contact with an infinite system characterized by the same Hamiltonian as defined in (1), for the CF we find:

$$\begin{aligned}
&\beta F_N^{\rm Cas}(K_s, K_l, h) := \qquad (12)\\
&\quad \beta f_\infty(K_s,K_l,h) + \frac{\partial}{\partial N}\ln Z_N(K_s,K_l,h) = \\
&\quad \beta f_\infty(K_s,K_l,h) + \frac{1}{2N} - \\
&\quad \frac{\int_{-\infty}^{\infty} dy\left(\Psi_p(y)e^{-N\Psi_p(y)} + \Psi_m(y)e^{-N\Psi_m(y)}\right)}{\int_{-\infty}^{\infty} dy\left(e^{-N\Psi_p(y)} + e^{-N\Psi_m(y)}\right)},
\end{aligned}$$

where the bulk free energy per spin is given by

$$\begin{aligned}
&\beta f_\infty(K_l,K_s,h) \qquad (13)\\
&= \begin{cases} \Psi_p\left(y_p^+|K_s,K_l,h\right), & \text{single minimum of } \Psi_p \\ 2\Psi_p\left(y_p^+ = y_p^-|K_s,K_l,h=0\right), & \text{two minima of } \Psi_p. \end{cases}
\end{aligned}$$

Then, provided Eq. (9) is valid, for the CCF we directly obtain

$$\beta F_N^{\rm Cas}(K_s,K_l,h) = \frac{1}{N} X_{\rm Cas}(x|K_s,K_l,h), \qquad (14)$$

where

$$\begin{aligned}
&X_{\rm N}^{\rm Cas}(x|K_s,K_l,h) = \\
&\quad -\frac{x\Upsilon(y_p^+,y_m^+)\exp[-x]}{1+\Phi(y_p^+,y_m^+)\exp[-x]}\left[1+\mathcal{O}(N^{-1})\right] < 0, \qquad (15)
\end{aligned}$$

with $x \equiv N\Phi(y_p^+,y_m^+)$. Thus, we derive that the CCF is *attractive* for all possible values of K_s, K_l and h. We recall that $\Psi_p(y_p^+|K_s,K_l,h) < \Psi_m(y_m^+|K_s,K_l,h)$, i.e., the force decays exponentially when $N \gg 1$; furthermore, the behavior of y_p^+ and y_m^+ as a function of K_s, K_l and h has to be determined from Eq. (7). We stress that the only dependence of the scaling function on N stems from the corresponding straightforward dependence of N in the scaling variable x. Finally, we recall that Eq. (14) is valid under the conditions which lead us to Eq. (9), namely that $\Psi_p^{(\rm II)}(y_p^+) > 0$ and $\Psi_m^{(\rm II)}(y_m^+) > 0$. It is easy to check, however, that at the critical line and also at the tricritical point this is no longer the case: at the line of the critical points $\Psi_p^{(\rm II)}(y_p^+ = 0) = 0$, while $\Psi_m^{(\rm II)}(y_m^+ = 0) = 1/K_l > 0$. Thus, Eq. (9) and Eq. (15) are no longer valid. Furthermore, one obtains $\Psi_p^{(\rm III)}(y_+) = 0$, while $\Psi_p^{(\rm IV)}(y_p^+ = 0) = e^{2K_s}\left(3e^{4K_s} - 1\right) > 0$ if the system is not positioned at the tricritical point. However, $\Psi_p^{(\rm IV)}(y_p^+ = 0) = 0$ at this point, while $\Psi_p^{(\rm VI)}(y_p^+ = 0|K_s = -\ln 3/4, K_l = \sqrt{3}/2, h = 0) = 4/\sqrt{3} > 0$. These facts lead to the following results:

i) The Casimir force at the critical line is:

$$\begin{aligned}
&\beta F_{\rm N}^{\rm Cas}(K_s, K_l = e^{-2K_s}/2, h = 0) \qquad (16)\\
&\quad = \frac{1}{N}\left\{\frac{1}{4} + \mathcal{O}\left[N^{-1/4}\exp[-2N\tanh^{-1}\left(e^{-2K_s}\right)]\right]\right\}.
\end{aligned}$$

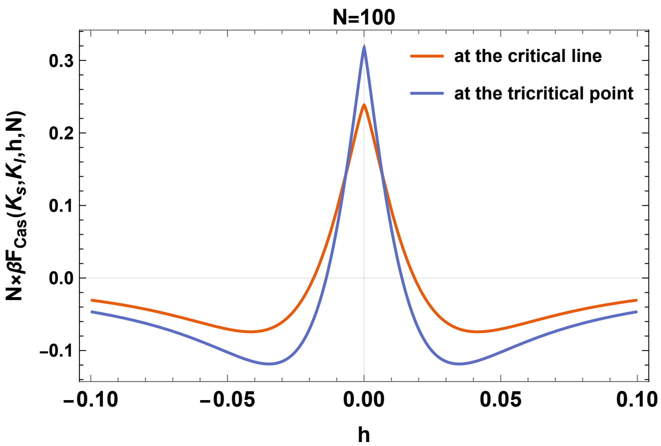

FIG. 2. The behavior of the CCF pertinent to NK model as a function of h for different fixed values of K_s and K_l with $N = 100$. The red line corresponds to $K_s = 0, K_l = 0.5$, while the blue line corresponds to the tricritical point which emerges in the phase diagram at coordinate $K_s = -\ln 3/4, K_l = \sqrt{3}/2$ obtained from the conditions: the multipliers in front of m^2 and m^4 equal zero, see Eq.(11). The results are in a full agreement with the derived exact results - see Eq. (16) and Eq. (17).

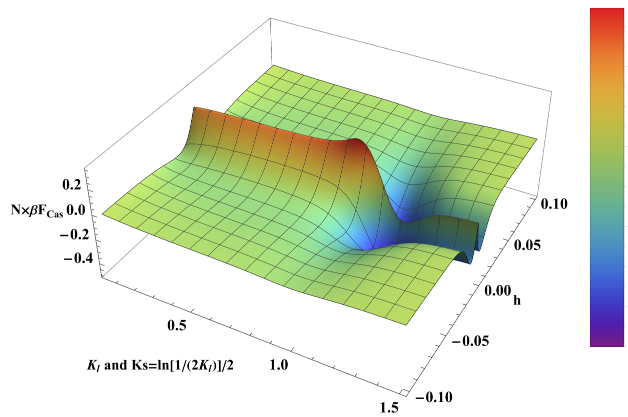

FIG. 3. The 3D visualization of the behavior of the CCF as a function of h for different fixed values of K_s and K_l with $N = 100$. Here $K_l \in (0, 1.5]$ while $K_s = \ln\left[1/(2K_l)\right]/2$ (i.e. on the line of the critical points). The results are in a full agreement with the derived exact results - see Eq. (16) and Eq. (17). As we see — despite the boundary conditions being periodic, in the framework of the NK model the CCF can be both repulsive and attractive, depending on the values of K_l, K_s and h. Obviously, the force is symmetric with respect to $h = 0$ as a function of h.

ii) At the tricritical point the following expression for the *tricritical* Casimir force (TCF) holds:

$$\beta F_{\rm N}^{\rm Cas}(K_s = -\ln 3/4, K_l = \sqrt{3}/2, h = 0) \tag{17}$$
$$= \frac{1}{N}\left\{\frac{1}{3} + \mathcal{O}\left[N^{-1/3}\exp\left[-2N\coth^{-1}\left(\sqrt{3}\right)\right]\right]\right\}.$$

iii) Close above $(+)$, or below $(-)$ the critical line:

$$\beta F_{\rm N}^{\rm Cas}(K_s, K_l, h = 0, N) = -\tfrac{1}{N}\sqrt{\tfrac{\pm[2K_l e^{2K_s}-1]N^{1/\nu_{\rm MF}}}{2K_l e^{2K_s}+1}}$$
$$\times \xi_I(K_s)^{-1}\exp\left[-N/\xi_I(K_s)\right]\left[1 + \mathcal{O}(N^{-1})\right]. \tag{18}$$

Here $\nu_{\rm MF} = 1/2$ and

$$\xi_I(K_s, h = 0) = \ln[\lambda_p/\lambda_m]^{-1} = -1/\ln[\tanh(K_s)] \tag{19}$$

is the correlation length (for $K_s \geq 0$ one has $\ln(\tanh(K_s)) < 0$) of the one-dimensional Ising model for $h = 0$ [33]. Thus, according to Eq. (18), the CCF close above or below the critical line is *attractive* and decays exponentially with $N \gg 1$. Let us note, however, that in the current problem we consider $K_s = O(1)$ along the line of critical points, i.e., $\xi_I = \mathcal{O}(1)$. Thus, in such a case $\left[2K_l e^{2K_s} - 1\right] N^{1/\nu_{\rm MF}}$ plays the role of a scaling variable.

iv) The case of nonzero external field, i.e., $h \neq 0$.

In this case the result for the CCF is given by Eq. (14) and Eq. (15). The force is *attractive*.

The general behavior of the CCF is numerically obtained and visualized in Figs. 2 and 3. We observe that the analytical expressions presented above confirm our analytical findings.

Conclusion: In the available literature on CCF's the following "boundary conditions rule" is widely accepted: in the whole range of temperatures, independently of the actual bulk universality class of the phase transition, the arising CCF is attractive for equal (symmetric) BC's [say, $(+,+)$, or $(0,0)$] and repulsive for unequal (asymmetric) BC's [say, antiperiodic or $(+,-)$] [34–36]. Indeed, the above statement is not a proven theorem, but an empirical finding that has been tested on a large number of models[35]. As we see, for the NK model under periodic boundary conditions this is *not* the case.

Our main results are:

- We have derived a closed-form analytic expression for the critical temperature of the second-order phase transition, $T_c(J_s, J_l)$, in terms of the Lambert W-function. This expression allows for the clarification of the behavior of the critical temperature as a function *simultaneously* of the two interaction constants K_s and K_l of the model (see Fig. 1).

- We show that the CCF is *repulsive* at the critical line and at the tricritical point, in spite of the applied periodic boundary conditions. The behavior of the *tricritical* Casimir force (TCF) is presented and compared with the standard CCF in Fig. 2. The exact Casimir amplitudes are: $\Delta_{\rm Cas}^{\rm (cr)} = 1/4$ at the critical line, and $\Delta_{\rm Cas}^{\rm (tr)} = 1/3$ at the tricritical point.

- Close to the critical line and the tricritical point the CF decays rapidly with distance away from them in the (temperature–field plane) - see Eq. (18). For $h \neq 0$ the

CF is attractive - see Eq. (15).

In essence, our main results are summarized, in form of 3-d behavior of the CCF, as a function of h for different fixed values of K_s and K_l, in Fig. 3. While the plot is in agreement with all analytical results stated above, we observe regions in which it is magnitude of the attraction exceeds that of its repulsion, when it is repulsive. Currently, we do not have analytical results for these regions.

Finally, we stress that the mechanism for changing the sign of the CCF is highly non-trivial and may not depend solely on whether the imposed boundary conditions are symmetrical or not. The beyond-mean-field model considered here shows that the 'boundary condition rule' is an incomplete statement and the presence of the competing interactions also matters. We note that a CCF with behavior that is repulsive or attractive, depending on the values of T and h has been also observed in the case of a ferromagnetic Ising ring with a competitive single antiferromagnetic bond [37].

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