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Alternative description of the 2D Blume–Capel model using Grassmann algebra

Maxime Clusel¹, Jean-Yves Fortin² and Vladimir N Plechko³

¹ Department of Physics and Center for Soft Matter Research, New-York University,

4 Washington place, NY 10003, USA

² Laboratoire de Physique Théorique, CNRS/UMR 7085 and Université Louis Pasteur,

3 rue de l'Université, 67084 Strasbourg cedex, France

³ Bogoliubov Laboratory of Theoretical Physics, Joint Institute for Nuclear Research, 141980 Dubna, Moscow Region, Russia

E-mail: mc2972@nyu.edu, fortin@lpt1.u-strasbg.fr and plechko@thsun1.jinr.ru

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Abstract

We use Grassmann algebra to study the phase transition in the two-dimensional ferromagnetic Blume–Capel model from a fermionic point of view. This model presents a phase diagram with a second-order critical line which becomes first order through a tricritical point. In particular, we are able to map the spin-1 system of the BC model onto an effective fermionic action from which we obtain the exact mass of the theory. The condition of vanishing mass defines the critical line. This effective action is actually an extension of the free fermion Ising action with an additional quartic interaction term. The effect of this term is merely to render the excitation spectrum of the fermions unstable at the tricritical point. The results are compared with recent numerical Monte Carlo simulations.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

The Blume–Capel (BC) model is a classical spin-1 model, originally introduced to study phase transitions in specific magnetic materials with a possible presence of non-magnetic states [1, 2]. Its modification was also used to qualitatively explain the phase transition in a mixture of He³–He⁴ adsorbed on a two-dimensional (2D) surface [3]. Below a concentration of 67% in He³, the mixture undergoes a so-called λ transition: the two components separate through a first-order phase transition and only He⁴ is superfluid. On a 2D lattice representing a helium film, He atoms are modelled by a spin-like variable, according to the following rule: a He³

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atom is associated to the value 0, whereas a He⁴ atom is represented by a classical Ising spin taking the values ± 1 . Within this framework, all the lattice sites are occupied either by a He³ or He⁴ atom [3]. The 2D Blume–Capel model describes the behaviour of this ensemble of spins $\{S_{mn} = 0, \pm 1\}$. In addition to the usual nearest-neighbour interaction, its energy includes the term $\Delta_0 \sum_{mn} S_{mn}^2$, with $S_{mn}^2 = 0, 1$, to take into account a possible change in the number of vacancies. Δ_0 can be thought of as a chemical potential for vacancies or as a parameter of the crystal field in a magnetic interpretation. A simple analysis of the 2D BC Hamiltonian already shows that this model presents a rather complex phase diagram in the plane (T, Δ_0) , where T is the temperature in the canonical ensemble [4]. In the limit $\Delta_0 \to -\infty$, the values $S_{mn} = 0$ are excluded and the standard 2D Ising model is recovered, with its well-known second-order critical point at $(T, \Delta_0) = (T_c = 2/\log(1 + \sqrt{2}) \simeq 2.269, -\infty)$, with the parameters taken in units of the Ising exchange energy J. At zero temperature, a simple energy argument shows that the ground state is the Ising like ordered state $|S_{mn}| = 1$ if $\Delta_0 < 2$, and $|S_{mn}| = 0$ else. There is therefore a first-order phase transition at $(T, \Delta_0) = (0, 2)$, suggesting a change in the order of the transition at some tricritical point of the critical line at finite temperature. Mean-field theory confirms this behaviour, and provides a second-order transition line in the plane (T, Δ_0) in the region $\Delta_0 < 0$, extending a little in the positive sector [1–5]. Beyond the tricritical point, as dilution increases, the transition becomes first order. Precise numerical simulations have been performed to study the phase diagram and to locate the tricritical point [6-10]. From theoretical backgrounds, several approximations have been used as well, such as mean-field theory [1-5], renormalization group analysis [11, 12] and high temperature expansions [13]. Using correlation identities and Griffith's and Newman's inequalities, rigorous upper bounds for the critical temperature have been obtained by Braga et al [14]. It was argued that exactly at the tricritical point the BC model falls into the conformal field theory (CFT) scheme of classification of the critical theories in two dimensions [15, 16]. This is the case m = 4 and c = 7/10, where c is the central charge [16, 17]. The CFT interpretation also implies a specific symmetry called super-symmetry in the 2D BC model at the tricritical point [17, 18]. The advanced theoretical methods like the bootstrap approach and perturbed conformal analysis in combination with integrable quantum field theory and numerical methods have been applied to study the scaling region and the RG flows in the 2D BC universality class [19–21].

The BC model is also directly related to percolation theory [22] and the dilute Potts model [23], where tricritical point properties are observed for percolating clusters of vacancies. We also mention quantitative results that match the universality class at the tricritical point of the BC model with that of a 2D spin fluid model representing a magnetic gas–fluid coexistence transition [24], or similarities between BC phase diagram and Monte Carlo results on the extended Hubbard model on a square lattice [25].

The aim of this paper is to present a different analytical method for the BC model in two dimensions with the use of the anti-commuting Grassmann variables, originally proposed for the classical 2D Ising model in the case of free fermions [26, 27] and since then used to treat various problems around the 2D Ising model, such as finite size effects and boundary conditions [28, 29], quenched disorder [30, 31], boundary magnetic field [32, 33]. In contrast with the use of traditional combinatorial and transfer-matrix considerations [34–36, 38], this method is rather based on a direct introduction of Grassmann variables (fermionic fields) into the partition function Z to decouple the spin degrees of freedom. A purely fermionic integral for Z then obtained by averaging on spin degrees of freedom in the resulting mixed spin-fermion representation for Z [26, 27]. This method turns out to be particularly efficient to deal with models with nearest-neighbour interactions in the 2D plane. For the 2D Ising model, the integral for Z appears to be a Gaussian integral over Grassmann variables. Respectively, the model is solvable and a Fourier transformation of the Grassmann variables in the action allows for a complete calculation of the partition function [37, 38]. In physical language, this corresponds to the case of free fermions [37, 38].

As the additional crystal field term in the BC Hamiltonian is local, we hoped that the method will be applicable as well in this context. Though it is not possible to compute exactly the partition function and thermodynamics quantities of the BC model directly, since the resulting fermionic action for BC is non-Gaussian, our approach allows to derive in a controlled way physical informations from the underlying fermionic lattice field theory with interaction. In the continuum limit, a simplified effective quantum field theory can be constructed and analysed in the low energy sector. The condition of vanishing mass leads to the exact equation for the critical line, and the effective interaction between fermions, to the existence of a tricritical point. The effects of interaction are analysed in the momentum-space representation. An approximate scheme such as Hartree-Fock-Bogoliubov (HFB) method can be used to locate the tricritical point. There are also some analogies, albeit rather formal, with approaches typically used in the context of BCS theory of ordinary superconductivity. In general, it is interesting to note that in 2D, a phase diagram of the BC model with first-order transition and tricritical point can be described not only with a bosonic Φ^6 Ginzburg–Landau theory where the order parameter is a simple scalar [39, 40], but also with the use of fermionic variables.

The paper is organized as follows. After presenting the BC Hamiltonian and the related partition function in standard spin-1 interpretation, we apply the fermionization procedure leading to the exact fermionic action on the lattice. We then derive the effective action in the continuum limit and extract the exact mass. The condition of zero mass already gives the equation for the critical line in the (T, Δ_0) plane. The effective action also includes four-fermion interaction due to the $S^2 = 0$ states (vacancies) in the system. We then give a physical interpretation for the existence of a tricritical point on the phase diagram, by studying the fermionic stability of the BC spectrum on the critical line at order k^2 in momentum. Our results are then compared with recent numerical Monte Carlo simulations [6–10].

2. The 2D Blume–Capel model

2.1. Hamiltonian and partition function

The 2D BC model is defined, on a square lattice of linear size L, via the following Hamiltonian:

$$H = -\sum_{m=1}^{L} \sum_{n=1}^{L} [J_1 S_{mn} S_{m+1n} + J_2 S_{mn} S_{mn+1}] + \Delta_0 \sum_{m=1}^{L} \sum_{n=1}^{L} S_{mn}^2.$$
(1)

In the above expression, $S_{mn} = 0, \pm 1$ is the BC spin-1 variable associated with the (m, n) lattice site coordinates, where m, n = 1, ..., L are running in the horizontal and vertical directions, respectively. The spins are interacting along the lattice bonds, $J_{1,2} > 0$ are the ferromagnetic exchange energies. In addition to the usual Ising spins with $S_{mn} = \pm 1$, there are as well non-magnetic sites $S_{mn} = 0$, which we shall also refer to as vacancies. The crystal field parameter Δ_0 plays the role of a chemical potential, being responsible for the level splitting between states $S_{mn} = 0$ and $S_{mn} = \pm 1$. The Hamiltonian that appears in the Gibbs exponential may be written in the form:

$$-\beta H = \sum_{m=1}^{L} \sum_{n=1}^{L} [K_1 S_{mn} S_{m+1n} + K_2 S_{mn} S_{mn+1}] + \Delta \sum_{m=1}^{L} \sum_{n=1}^{L} S_{mn}^2, \qquad (2)$$

where $K_{1,2} = \beta J_{1,2}$ are now the temperature dependent coupling parameters, $\beta = 1/T$ is inverse temperature in the energy units, and $\Delta = -\beta \Delta_0$. In the following we mainly

focus on the ferromagnetic case, with positive $J_{1,2} > 0$ and $K_{1,2} > 0$. Note however that the fermionization procedure by itself is valid irrespective of the signs of interactions.⁴ The positive Δ (negative Δ_0) is favourable for the appearance of the Ising states in the system, with the ordered phase below the critical line in the (T, Δ_0) plane, at low temperatures, while negative Δ (positive Δ_0) will suppress Ising states, being favourable for vacancies. In the limit $\Delta_0 \rightarrow -\infty$ (or $\Delta \rightarrow +\infty$) the states with $S_{mn}^2 = 0$ are effectively suppressed and the model reduces to the 2D Ising model, with the critical temperature being defined by the condition $\sinh 2K_1 \sinh 2K_2 = 1$. As Δ_0 increases to finite values, there will be a line of phase transitions in the (T, Δ_0) plane. The critical line goes to lower temperatures as parameter Δ_0 increases and terminates at $\Delta_0 = J_1 + J_2$ at zero temperature, so that all sites are empty at larger positive values of Δ_0 at T = 0. A remarkable feature of the BC model is that there is also a tricritical point on the critical line somewhere slightly to the left from $\Delta_0 = J_1 + J_2$, where the transition changes from second to first order.

The partition function Z of the BC model is obtained by summing over all possible spin configurations at each site, $Z = \sum_{\{S_{mn}=0,\pm1\}} e^{-\beta H} \equiv \operatorname{Tr}_{\{S\}} e^{-\beta H}$. It is easy to develop each Boltzmann factor appearing in the above trace formula in a polynomial form:

$$\exp(K_i SS') = 1 + \lambda_i SS' + \lambda'_i S^2 S'^2, \qquad i = 1, 2,$$
(3)

with

$$\lambda_i = \sinh K_i, \qquad \lambda'_i = \cosh K_i - 1, \qquad i = 1, 2. \tag{4}$$

The partition function is then given by the trace of the product of above spin-polynomial Boltzmann weights:

$$Z = \prod_{\{S_{mn}=0,\pm1\}} \left\{ \prod_{m=1}^{L} \prod_{n=1}^{L} e^{\Delta S_{mn}^{2}} \left[\left(1 + \lambda_{1} S_{mn} S_{m+1n} + \lambda_{1}' S_{mn}^{2} S_{m+1n}^{2} \right) \right. \\ \left. \times \left(1 + \lambda_{2} S_{mn} S_{mn+1} + \lambda_{2}' S_{mn}^{2} S_{mn+1}^{2} \right) \right] \right\}.$$
(5)

This expression will be the starting point of the fermionization procedure for Z using Grassmann variables we develop in section 3. As a first step we introduce new Grassmann variables to decouple the spins in the local polynomial factors of expression (5). The second step is to sum over spin states in the resulting mixed spin-fermion representation for Z to obtain a purely fermionic theory for Z.

2.2. Local spin decomposition

In what follows, we need to average partially fermionized Z over the spin states at each site. This averaging will be performed in two steps, first we keep in mind to average over the Ising degrees of freedom, $S_{mn} = \pm 1$, then adding the contribution of vacancies, $S_{mn} = 0$. The two cases may be also distinguished in terms of variable $S_{mn}^2 = 0$, 1. In this subsection, we make a comment on the formalization of this two-step averaging. Provided we have any function of the BC spin-1 variable $f(S_{mn})$, with $S_{mn} = 0, \pm 1$, the averaging rule is simple:

$$\sum_{S_{mn}=0,\pm 1} f(S_{mn}) = f(0) + f(+1) + f(-1).$$
(6)

⁴ In what follows, making approximations in the resulting fermionic integrals, and by presenting the numerical results, we shall typically assume the isotropic case in the above Hamiltonians, with $J = J_1 = J_2$, $K = K_1 = K_2$ and $K = \beta J$. We will also use, in some cases, the dimensionless parameters normalized by the exchange energy J for temperature T and chemical potential Δ_0 .

S.

In forthcoming procedures, we ought to average first over the states $S_{mn} = \pm 1$ at each site, provided $S_{mn}^2 = 1$, while making the sum over choices $S_{mn}^2 = 0$, 1 at next stage. In principle, since $S_{mn} = \text{sign}\{S_{mn}\}|S_{mn}|$, with $\text{sign}\{S_{mn}\} = \pm 1$ and $|S_{mn}| = S_{mn}^2 = 0$, 1, we can try simply to write $S_{mn} = y_{mn}\sigma_{mn}$, where $y_{mn} = 0$, 1, and $\sigma_{mn} = \pm 1$, and to average over the component states $y_{mn} = 0$, 1 and $\sigma_{mn} = \pm 1$ as independent variables. This gives:

$$\sum_{y_{mn}=0,1;\sigma_{mn}=\pm 1} f(y_{mn}\sigma_{mn}) = f(+0) + f(-0) + f(+1) + f(-1).$$
(7)

We see that the zero state is counted twice, in contradiction to (6). This may be corrected by introducing in the definition of the averaging the weight factor $\frac{1}{2}$ at $y_{mn} = 0$. Equivalently, this may be done by adding $2^{-1+y_{mn}}$ under the sum. This results the sum of three terms in agreement with (6):

$$\sum_{mn=0,1;\sigma_{mn}=\pm 1} 2^{-1+y_{mn}^2} f(\sigma_{mn}y_{mn}) = f(0) + f(+1) + f(-1).$$
(8)

In fact, this decomposition scheme with $S_{mn} = \sigma_{mn} y_{mn}$ and independently varying $\sigma_{mn} = \pm 1$ and $y_{mn} = 0, 1$ is somewhat more close to the situation for the two-dimensional Ising model with quenched site dilution [30, 31]. In that case $\sigma_{mn} = \pm 1$ is simply the Ising spin, while the variable $y_{mn} = 0, 1$ is the quenched dilution parameter, counting whether the given site is occupied or dilute, and both averaging rules (7) and (8) can be interpreted physically. The case (7) means simply that there is a spin $\sigma_{mn} = \pm 1$ also at site $y_{mn} = 0$, which is not interacting with its nearest neighbours. This empty, or rather disconnected, site, by flipping over two states ± 1 under temperature fluctuations, will give however a contribution to the entropy, ln 2 by empty site. Case (8) means that the site $y_{mn} = 0$ is really dilute, or empty, with no spin degree of freedom at it, even disconnected.

For the quenched dilute 2D Ising model, the quenched averaging over some fixed temperature-independent distribution $y_{mn} = 0$, 1 is distinct from the $\sigma_{mn} = \pm 1$ averaging, and is assumed to be performed on $-\beta F = \ln Z$, but not on Z itself. The situation is different for the BC model, which is rather the annealed case of the site dilute Ising model, with averaging simultaneously over all the states $S_{mn} = 0, \pm 1$ at each site for Z itself. In this case the averaging is to be performed strictly according to the rules of (6) and (8), but not (7).

There is still another way to formalize the averaging over the possibilities $S_{mn} = \pm 1$ before we actually perform the sums $S_{mn}^2 = 0$, 1. It is based on the observation that the result of the averaging (6) will not be changed if we replace $S_{mn} \rightarrow \sigma_{mn}S_{mn}$, with $\sigma_{mn} = \pm 1$, since the sum includes $S_{mn} = \pm 1$ anyhow

$$\sum_{S_{mn}=0,\pm 1} f(S_{mn}) = \sum_{S_{mn}=0,\pm 1} f(\sigma_{mn}S_{mn}) = f(0) + f(+1) + f(-1), \sigma_{mn} = \pm 1.$$
(9)

Though the above equation holds already for any fixed value of $\sigma_{mn} = \pm 1$, we can as well average it over the states $\sigma_{mn} = \pm 1$, introducing factor $\frac{1}{2}$ for normalization. The averaging of $f(\sigma_{mn}S_{mn})$ itself gives

$$\frac{1}{2}\sum_{\sigma_{mn}=\pm 1} f(\sigma_{mn}S_{mn}) = \frac{1}{2}[f(S_{mn}) + f(-S_{mn})] = g(S_{mn}^2), \qquad S_{mn}^2 = 0, 1.$$
(10)

The result of the averaging will be a function g which only depends on $|S_{mn}| = 0, 1$, alias $S_{mn}^2 = 0, 1$, but not on the sign $\{S_{mn}\}$. In terms of $g(S_{mn}^2)$, equation (9) results

$$\sum_{nn=0,\pm 1} f(S_{mn}) = \sum_{S_{mn}=0,\pm 1} \left\{ \frac{1}{2} \sum_{\sigma_{mn}=\pm 1} f(\sigma_{mn}S_{mn}) \right\} = g(0) + 2g(1).$$
(11)

In this form the two-step averaging will be realized in the procedure of elimination of spin variables by constructing the fermionic integral for *Z* in the forthcoming discussion.

3. Fermionization and lattice fermionic field theory

The expression of the BC partition function Z as a product of spin polynomials under the averaging as given in (5) will be the starting point of the fermionization procedure for Z. This procedure has first been introduced in the context of the 2D pure Ising model [26, 27]. It relies on interpreting each spin polynomial Boltzmann weight in (5) as the result of integration over a set of two Grassmann variables, which decouples the spins under the integral. Before going into details, we remind in the following subsection few essential features about Grassmann variables and the rules of integration.

3.1. Grassmann variables

Mathematically, Grassmann variables may be viewed as formal purely anti-commuting numbers [41]. In physical aspect, they are images of quantum fermions in path integral [41]. Let us remember few basic rules for Grassmann variables that are needed in the rest of the paper. More details can be found in [42, 43].

A Grassmann algebra A of size N is generated by a set of N anti-commuting objects $\{a_1, a_2, \ldots, a_N\}$ satisfying

$$a_i a_j + a_j a_i = 0,$$
 $a_i^2 = 0,$ $i, j = 1, 2, \dots, N.$ (12)

Unlike quantum fermions, Grassmann variables are totally anti-commuting. Note that any linear superpositions of the original variables (12) are again purely anti-commuting, with each other and with the original variables. Their squares are zeros too. Functions defined on such an algebra are particularly simple, they are always polynomials with a finite degree (since $a_i^2 = 0$). It is possible to define the notion of integration in algebra of such polynomials with the following rules [41]:

$$\int \mathrm{d}a_i \cdot a_i = 1, \qquad \int \mathrm{d}a_i \cdot 1 = 0. \tag{13}$$

Integral with many variables is considered as a multilinear functional with respect to each of the variables involved into integration. In multiple integrals, the fermionic differentials are again anti-commuting with each other and the variables themselves. The integration of any polynomial function of Grassmann variables like $f(a) = f(a_1, a_2, ..., a_N)$ then reduces, in principle, to a repeating use of the above rules.

The rules of change of variables in Grassmann variable (fermionic) integrals under a linear substitution are similar to the analogous rules of common commuting analysis. The only difference is that the Jacobian of the transformation will enter now in the inverse power, contrarily to the commuting (bosonic) case [40–43].

With the above definitions, Gaussian integrals over Grassmann variables are all expressed by equations relating them to determinants and Pfaffians. The basic identity for the integral of first kind reads

$$\int \prod_{i=1}^{N} \mathrm{d}a_i^* \mathrm{d}a_i \exp\left(\sum_{i,j=1}^{N} a_i A_{ij} a_j^*\right) = \det A, \tag{14}$$

where the integration is over the doubled set of totally anti-commuting variables $\{a, a^*\}$, the (square) matrix A in the exponential being arbitrary. In applications, quadratic fermionic form in the exponential like in (14) is typically called *action*. Since the action is quadratic, the integral is Gaussian. Since the action is quadratic, the integral is Gaussian.

in (14) is assumed in the sense of its series expansion. Due to nilpotent properties of fermions, the exponential series definitely terminates at some stage, thus resulting a finite polynomial in variables involved under the integral. (With respect to the action $S = aAa^*$ taken as a whole, the last nonzero term will be with $S^N \neq 0$, while $S^{N+1} = 0$. Alternatively, the same polynomial for the exponential from (14) will follow by multiplying elementary factors like $\exp(a_i A_{ij}a_j^*) = 1 + a_i A_{ij}a_j^*$). In physical interpretation, the integral of the first kind (14) with complex-conjugate fields rather corresponds to Dirac theories. The Majorana theories with real fermionic fields are presented by the Gaussian integrals of the second kind related to the Pfaffian. The fermionic integral of the second kind reads

$$\int \prod_{i=1}^{\infty} \mathrm{d}a_i \exp\left(\sum_{i,j=1}^N \frac{1}{2} a_i A_{ij} a_j\right) = \mathrm{Pf} A.$$
(15)

The integration is over the set of even number *N* of Grassmann variables. Arrow in the measure indicates the direction of ordering of the anti-commuting differentials. Due to anti-commutation relations the matrix in the exponential is now assumed skew-symmetric, with $A_{ij} + A_{ji} = 0$, and $A_{ii} = 0$. The result of integration is the Pfaffian associated with the skew-symmetric matrix *A*. In physics, the combinatorics of the Pfaffian also is well known under the name of the (fermionic) Wick's theorem.

In a combinatorial sense, the determinant is actually a particular case of the Pfaffian. Respectively, the integral (14) is a subcase of the integral (15). It can be shown that $(PfA)^2 = \det A$ for any skew-symmetric matrix A. This implies that in principle, an integral of the second kind (15) can always be reduced to an integral of first kind (14) by doubling the number of fermions in (15). In applications like in the Ising and BC models where the original integrals in the real lattice space naturally appear in the Pfaffian like form of (15), this reduction to the first case occurs automatically after transformation to the momentum space, where the fermionic variables are typically combined into groups of variables with opposite momenta (k, -k), which play the role of the conjugated variables like in (14). In practice however, for low-dimensional integrals, most of calculations can be performed simply from the definition of the integral, by expanding the integrand functions into polynomials.

3.2. Fermionization procedures

In the same spirit as for the 2D Ising model [27], we introduce two pairs of Grassmann variables per site (a_{mn}, \bar{a}_{mn}) , and (b_{mn}, \bar{b}_{mn}) to factorize the polynomials appearing in (5). Namely we use the relations

$$1 + \lambda_{1} S_{mn} S_{m+1n} + \lambda_{1}' S_{mn}^{2} S_{m+1n}^{2} = \int d\bar{a}_{mn} da_{mn} e^{(1+\lambda_{1}' S_{mn}^{2} S_{m+1n}^{2})a_{mn}\bar{a}_{mn}} \\ \times (1 + a_{mn} S_{mn})(1 + \lambda_{1}\bar{a}_{mn} S_{m+1n}), \\ 1 + \lambda_{2} S_{mn} S_{mn+1} + \lambda_{2}' S_{mn}^{2} S_{mn+1}^{2} = \int d\bar{b}_{mn} db_{mn} e^{(1+\lambda_{2}' S_{mn}^{2} S_{mn+1}^{2})b_{mn}\bar{b}_{mn}} \\ \times (1 + b_{mn} S_{mn})(1 + \lambda_{2}\bar{b}_{mn} S_{mn+1}).$$
(16)

For the sake of simplicity in the notation, let us introduce the following link factors:

$$A_{mn} = 1 + a_{mn}S_{mn}, \qquad \bar{A}_{m+1n} = 1 + \lambda_1 \bar{a}_{mn}S_{m+1n}, B_{mn} = 1 + b_{mn}S_{mn}, \qquad \bar{B}_{mn+1} = 1 + \lambda_2 \bar{b}_{mn}S_{mn+1}.$$
(17)

We also define the Grassmann local trace operators which associate with any function f on the Grassmann algebra as follows:

$$\begin{aligned} \mathfrak{Tr}_{(a_{mn})}[f(a_{mn},\bar{a}_{mn})] &= \int d\bar{a}_{mn} \, da_{mn} \, \mathrm{e}^{(1+\lambda'_{1}S^{2}_{mn}S^{2}_{m+1n})a_{mn}\bar{a}_{mn}} \, f(a_{mn},\bar{a}_{mn}), \\ \mathfrak{Tr}_{(b_{mn})}[f(b_{mn},\bar{b}_{mn})] &= \int d\bar{b}_{mn} \, \mathrm{d}b_{mn} \, \mathrm{e}^{(1+\lambda'_{2}S^{2}_{mn}S^{2}_{mn+1})b_{mn}\bar{b}_{mn}} \, f(b_{mn},\bar{b}_{mn}). \end{aligned}$$
(18)

The factorized Boltzmann weights from (16) then read:

$$1 + \lambda_1 S_{mn} S_{m+1n} + \lambda_1' S_{mn}^2 S_{m+1n}^2 = \underset{(a_{mn})}{\mathfrak{Tr}} [A_{mn} \bar{A}_{m+1n}],$$

$$1 + \lambda_2 S_{mn}^2 S_{mn+1}^2 + \lambda_2' S_{mn}^2 S_{mn+1}^2 = \underset{(b_{mn})}{\mathfrak{Tr}} [B_{mn} \bar{B}_{mn+1}].$$
(19)

Introducing the above Grassmann factors into the original expression (5) for *Z*, we obtain a mixed representation containing both spins and Grassmann variables for *Z*. Note that as the separable link factors like A_{mn} , \bar{A}_{mn} , B_{mn} , \bar{B}_{mn} are neither commuting or anti-commuting with each other, the order in which they appear in the product may be important. The factorized bond weights, however, presented in (19) by doubled link factors under the trace operators, are totally commuting, if taken as a whole, with any element of the algebra under the averaging. For the whole lattice, we define the global trace operator as follows:

$$\mathfrak{Tr}_{(a,b)}[f] = \int \prod_{m=1}^{L} \prod_{n=1}^{L} d\bar{a}_{mn} \, da_{mn} \, d\bar{b}_{mn} \, db_{mn} \, e^{\Delta S_{mn}^2} f(a_{mn}, \bar{a}_{mn}, b_{mn}, \bar{b}_{mn}) \\ \times \exp\left\{\sum_{m=1}^{L} \sum_{n=1}^{L} \left[\left(1 + \lambda_1' S_{mn}^2 S_{m+1n}^2\right) a_{mn} \bar{a}_{mn} + \left(1 + \lambda_2' S_{mn}^2 S_{mn+1}^2\right) b_{mn} \bar{b}_{mn} \right] \right\}.$$
(20)

The all even-power terms in spin variables are now incorporated into the generalized Gaussian averaging measure of (20), including the term with chemical potential. The partition function is given by

$$Z = \operatorname{Tr}_{\{S\}} \mathfrak{Tr}_{(a,b)} \left[\prod_{n=1}^{\overrightarrow{L}} \left(\prod_{m=1}^{\overrightarrow{L}} ((A_{mn} \overline{A}_{m+1n}) (B_{mn} \overline{B}_{mn+1})) \right) \right].$$
(21)

At this stage the factorized partition function appears as a double trace, over the spin degrees of freedom, with $Tr_{\{S\}}$, and over the Grassmann variables, with $\mathfrak{Tr}_{(a,b)}$. The idea of the next step is to make spin summation in (21) to obtain a purely fermionic integral for *Z*.

3.3. The ordering of factors

Up to now we have only added extra Grassmann variables to obtain the mixed expression (21) where the spin variables are actually decoupled into separable link factors like (17). Further algebraic manipulations are necessary to simplify this expression in order for the spin averaging to be possible in each group of factors with the same spin. For any given *mn*, there are four such factors, A_{mn} , \bar{B}_{mn} , \bar{A}_{mn} , \bar{B}_{mn} , which all include the same BC spin $S_{mn} = 0, \pm 1$. We apply the mirror-ordering procedure [26, 27] to move together, whenever possible, the different link factors containing the same spin. Separable link factors like (17) are in general neither commuting nor anti-commuting with each other. Doubled combinations representing the bond weights in (19) like $A_{mn}\bar{A}_{m+1n}$ or $B_{mn}\bar{B}_{mn+1}$, are however effectively commuting with any element of the algebra, if taken as a whole: commutation does not change the results

of the Gaussian fermionic averaging (20). We use mirror-ordering decoupling for factors in vertical direction, $B_{mn}\bar{B}_{mn+1}$, with respect to *n*, insert the commuting factorized horizontal weights, $A_{mn}\bar{A}_{m+1n}$, and reread the resulting products in few subsequent transformations [26, 27]. This leads to

$$Z = \operatorname{Tr} \mathfrak{Tr} \left\{ \prod_{m=1}^{L} \prod_{n=1}^{L} \left[(A_{mn} \bar{A}_{m+1n}) (B_{mn} \bar{B}_{mn+1}) \right] \right\},$$

$$= \operatorname{Tr} \mathfrak{Tr} \left\{ \prod_{n=1}^{L} \left[\prod_{m=1}^{L} \bar{B}_{mn} A_{mn} \bar{A}_{m+1n} \cdot \prod_{m=1}^{L} B_{mn} \right] \right\},$$

$$= \operatorname{Tr} \mathfrak{Tr} \left\{ \prod_{n=1}^{L} \left(\left(\prod_{m=1}^{L} \bar{A}_{mn} \bar{B}_{mn} A_{mn} \right) \cdot \left(\prod_{m=1}^{L} B_{mn}, \right) \right) \right\}.$$
(22)

Going from (21) to (22) one has to pay attention to boundary terms. The simplest case corresponds to free boundary conditions for spin variables, $S_{L+1n} = S_{mL+1} = 0$ in (5): it corresponds to free boundary conditions for fermions, $\bar{a}_{0n} = \bar{b}_{m0} = 0$, in (22). For these boundary conditions, the transformation from (21) to (22) is actually exact. In the following however, we will typically use periodic boundary conditions for fermions in representations like (22), which are suitable when passing to the Fourier space for anti-commuting (Grassmann) fields. The change of the boundary conditions is inessential anyway in the limit of infinite lattice, $L \to \infty$. In principle, one can pay more attention to the effects of the boundary terms in the periodic case, which can actually be treated rigorously for finite lattices [27, 29, 32, 33].

In the case of the 2D Ising model, with $S_{mn}^2 = 1$, we can explicitly perform the trace over the Ising spin degrees of freedom $S_{mn} = \pm 1$ recursively at the junction of two *m*-ordered products in the final line of (22). The situation is slightly different in the BC case: trace operator (20) contains terms with $S_{mn}^2 = 0$, 1 which are coupled at neighbouring sites. Therefore it is not possible to trace over the whole set of states $S_{mn} = 0, \pm 1$ in the BC case directly in (22). We can eliminate first the Ising degrees $\sigma_{mn} = \text{sign}\{S_{mn}\} = \pm 1$. The occupancy variables $S_{mn}^2 = 0, 1$ will still remain as parameters and will be eliminated at next stages.

3.4. Spin summation

At the junction of the two ordered products in (22), with $S_{mn} \rightarrow \sigma_{mn}S_{mn}$, we perform the trace $\sigma_{mn} = \pm 1$ recursively, for $m = L, L-1, \ldots, 2, 1$, for any given *n*, starting with m = L. The procedure will then be repeated for other values of $n = 1, 2, \ldots, L$. We recover then the four factors \bar{A}_{mn} , \bar{B}_{mn} , A_{mn} , B_{mn} (17), with the same spin that met at the junction of the two *m*-product in (22), for given *n*. Then we multiply the above four factors, taking also into account that $\sigma_{mn}^2 = 1$, so that $S_{mn}^2 \rightarrow \sigma_{mn}^2 S_{mn}^2 \rightarrow S_{mn}^2$, and sum over the states $\sigma_{mn} = \pm 1$. This will eliminate all odd terms in the polynomial so obtained. The averaging leads to

$$\frac{1}{2} \sum_{\sigma_{mn}=\pm 1} \bar{A}_{mn} \bar{B}_{mn} A_{mn} B_{mn} \\
= 1 + S_{mn}^2 a_{mn} b_{mn} + S_{mn}^2 (\lambda_1 \bar{a}_{m-1n} + \lambda_2 \bar{b}_{mn-1}) (a_{mn} + b_{mn}) \\
+ S_{mn}^2 \lambda_1 \lambda_2 \bar{a}_{m-1n} \bar{b}_{mn-1} + S_{mn}^4 \lambda_1 \lambda_2 a_{mn} b_{mn} \bar{a}_{m-1n} \bar{b}_{mn-1}, \\
= \exp \left[S_{mn}^2 (a_{mn} b_{mn} + (\lambda_1 \bar{a}_{m-1n} + \lambda_2 \bar{b}_{mn-1}) (a_{mn} + b_{mn}) + \lambda_1 \lambda_2 \bar{a}_{m-1n} \bar{b}_{mn-1}) \right]. \tag{23}$$

The resulting even fermionic polynomial can be written as a Gaussian exponential, as shown in the final line. This term is totally commuting with all other elements of the algebra and can be removed outside of the junction. The BC spins still remain in the form of $S_{mn}^2 = 0, 1$ in (23), but the Ising degrees, $\sigma_{mn} = \pm 1$, are already eliminated. After completing the above averaging procedure at the junction at m = L, we repeat the calculation for m = L - 1, ..., 1, for given n, and then for other values of n = 1, ..., L. Adding the diagonal terms from the definition of the fermionic averaging (20), the partially traced partition function finally reads

$$Z = 2^{L^{2}} \operatorname{Tr}_{\{S^{2}=0,1\}} \int \prod_{m,n=1}^{L} d\bar{a}_{mn} da_{mn} d\bar{b}_{mn} db_{mn} \exp\left[\Delta S_{mn}^{2} + \left(1 + \lambda_{1}' S_{mn}^{2} S_{m+1n}^{2}\right) a_{mn} \bar{a}_{mn} + \left(1 + \lambda_{2}' S_{mn}^{2} S_{m+1n}^{2}\right) b_{mn} \bar{b}_{mn} + S_{mn}^{2} (\lambda_{1} \bar{a}_{m-1n} + \lambda_{2} \bar{b}_{mn-1}) (a_{mn} + b_{mn}) + S_{mn}^{2} a_{mn} b_{mn} + S_{mn}^{2} \lambda_{1} \lambda_{2} \bar{a}_{m-1n} \bar{b}_{mn-1}\right].$$
(24)

The resulting integral for Z in (24) is a Gaussian integral, which includes the variables $S_{mn}^2 = 0, 1$ as parameters. At this stage, it is easy to recognize that the 2D Ising model is solvable: in this case $S_{mn}^2 = 1$ for all sites, so that the partition function (24) no longer contains spin degrees of freedom. It can then be readily evaluated by passing to the momentum space [26, 27]. In the BC model case, it remains yet to eliminate $S_{mn}^2 = 0, 1$ degrees of freedom in the above expression (24). This can be performed after we manage to decouple the variables in terms including $S_{mn}^2 S_{m+1n}^2$ and $S_{mn}^2 S_{mn+1}^2$. Several methods are possible. One way is to introduce another auxiliary set of Grassmann link variables, similarly to what we previously did to decouple the factors $S_{mn} S_{m+1n}$ and $S_{mn} S_{mn+1}$ in (16). It is possible however to avoid the introduction of the new fields by performing the following change of Grassmann variables in (24): $a_{mn} \to a_{mn}/S_{mn}^2$, $b_{mn} \to b_{mn}/S_{mn}^2$, $d_{mn} \to S_{mn}^2 d_{mn}$, $d_{mn} \to S_{mn}^2 d_{mn}$. The variable S_{mn}^2 then disappears in some places inside the exponential and appears in others, the terms with $S_{mn}^2 S_{m+1n}^2$ and $S_{mn}^2 S_{mn}^2 + b_{mn}/S_{mn}^2$ are to be understood as $S_{mn}^2 \exp(a_{mn}\bar{a}_{mn}/S_{mn}^2) = S_{mn}^2(1 + a_{mn}\bar{a}_{mn}/S_{mn}^2) = S_{mn}^2 + a_{mn}\bar{a}_{mn}$. Finally, after shifting some indices in the total mn sums in the exponential, we obtain

$$Z = 2^{L^{2}} \operatorname{Tr}_{\{S^{2}=0,1\}} \int \prod_{m,n=1}^{L} d\bar{a}_{mn} da_{mn} d\bar{b}_{mn} db_{mn} \left(S_{mn}^{2} + a_{mn}\bar{a}_{mn}\right) \left(S_{mn}^{2} + b_{mn}\bar{b}_{mn}\right)$$

$$\times \exp\left[\Delta S_{mn}^{2} + S_{mn}^{2} (\lambda_{1}'a_{m-1n}\bar{a}_{m-1n} + \lambda_{2}'b_{mn-1}\bar{b}_{mn-1} + \lambda_{1}\lambda_{2}\bar{a}_{m-1n}\bar{b}_{mn-1})\right]$$

$$\times \exp\left[a_{mn}b_{mn} + (\lambda_{1}\bar{a}_{m-1n} + \lambda_{2}\bar{b}_{mn-1})(a_{mn} + b_{mn})\right]. \tag{25}$$

In this expression, we can already locally perform the sum over $S_{mn}^2 = 0$, 1 at each site, using rules like (8) in order to avoid counting twice the contribution of $S_{mn}^2 = 0$ states

$$\sum_{\{S_{mn}^{2}=0,1\}} \left\{ 2^{S_{mn}^{2}} \left[\left(S_{mn}^{2} + a_{mn}\bar{a}_{mn} \right) \left(S_{mn}^{2} + b_{mn}\bar{b}_{mn} \right) \right] \\ \times \exp \left[S_{mn}^{2} \left(\Delta + \lambda_{1}' a_{m-1n}\bar{a}_{m-1n} + \lambda_{2}' b_{mn-1}\bar{b}_{mn-1} + \lambda_{1}\lambda_{2}\bar{a}_{m-1n}\bar{b}_{mn-1} \right) \right] \right\} \\ = a_{mn}\bar{a}_{mn}b_{mn}\bar{b}_{mn} + 2e^{\Delta}e^{G_{mn}}.$$
(26)

The first term is that produced at dilute site with $S_{mn}^2 = 0$. The polynomial G_{mn} in final line stands for the local part of the action resulting at the Ising site with $S_{mn}^2 = 1$

$$G_{mn} = a_{mn}\bar{a}_{mn} + b_{mn}\bar{b}_{mn} + \lambda_1\lambda_2\bar{a}_{m-1n}\bar{b}_{mn-1} + \lambda'_1a_{m-1n}\bar{a}_{m-1n} + \lambda'_2b_{mn-1}\bar{b}_{mn-1}.$$
 (27)

The result of the averaging from (26) can as well be written as a unique exponential taking into account the nilpotent property of fermions

$$a_{mn}\bar{a}_{mn}b_{mn}\bar{b}_{mn} + 2e^{\Delta}e^{G_{mn}} = 2e^{\Delta}e^{G_{mn}}\left(1 + \frac{1}{2}a_{mn}\bar{a}_{mn}b_{mn}\bar{b}_{mn}e^{-\Delta - G_{mn}}\right)$$

= $2e^{\Delta}\exp\left(G_{mn} + \frac{1}{2}a_{mn}\bar{a}_{mn}b_{mn}\bar{b}_{mn}e^{-\Delta - G_{mn}}\right)$
= $2e^{\Delta}\exp\left(G_{mn} + \frac{1}{2}e^{-\Delta}a_{mn}\bar{a}_{mn}b_{mn}\bar{b}_{mn}e^{-G'_{mn}}\right).$ (28)

with

$$G'_{mn} = \lambda'_1 a_{m-1n} \bar{a}_{m-1n} + \lambda'_2 b_{mn-1} \bar{b}_{mn-1} + \lambda_1 \lambda_2 \bar{a}_{m-1n} \bar{b}_{mn-1}.$$
 (29)

Substituting this result into (25) and shifting the mn index once again in some of the diagonal terms of the resulting combined action, we obtain

$$Z = 2^{L^{2}} e^{L^{2}\Delta} \int \prod_{m=1}^{L} \prod_{n=1}^{L} d\bar{a}_{mn} da_{mn} d\bar{b}_{mn} db_{mn} \exp\left\{\sum_{m=1}^{L} \sum_{n=1}^{L} [(1 + \lambda_{1}')a_{mn}\bar{a}_{mn} + (1 + \lambda_{2}')b_{mn}\bar{b}_{mn} + a_{mn}b_{mn} + (\lambda_{1}\bar{a}_{m-1n} + \lambda_{2}\bar{b}_{mn-1})(a_{mn} + b_{mn}) + \lambda_{1}\lambda_{2}\bar{a}_{m-1n}\bar{b}_{mn-1} + \bar{g}_{0}a_{mn}\bar{a}_{mn}b_{mn}\bar{b}_{mn} \exp(-\lambda_{1}'a_{m-1n}\bar{a}_{m-1n} - \lambda_{2}'b_{mn-1}\bar{b}_{mn-1} - \lambda_{1}\lambda_{2}\bar{a}_{m-1n}\bar{b}_{mn-1})]\right\},$$
(30)

with

$$\bar{g}_0 = \mathrm{e}^{-\Delta}/2, \qquad \Delta = -\beta \Delta_0.$$
 (31)

This is already a purely fermionic integral for Z, since spin degrees of freedom being completely eliminated. To simplify the comparison with the 2D Ising model and for other needs, we may rescale some of the Grassmann variables under the integral using the following transformation:

$$(1+\lambda_1')\bar{a}_{mn} \to \bar{a}_{mn}, \qquad (1+\lambda_2')\bar{b}_{mn} \to \bar{b}_{mn}. \tag{32}$$

The corresponding differentials are to be rescaled with inverse factors. In this way, we obtain the final result

$$Z = (2 e^{\Delta} \cosh K_{1} \cosh K_{2})^{L^{2}} \int \prod_{m=1}^{L} \prod_{n=1}^{L} d\bar{a}_{mn} da_{mn} d\bar{b}_{mn} db_{mn}$$

$$\times \exp\left\{\sum_{m=1}^{L} \sum_{n=1}^{L} \left[a_{mn}\bar{a}_{mn} + b_{mn}\bar{b}_{mn} + a_{mn}b_{mn} + (t_{1}\bar{a}_{m-1n} + t_{2}\bar{b}_{mn-1})(a_{mn} + b_{mn}) + t_{1}t_{2}\bar{a}_{m-1n}\bar{b}_{mn-1} + g_{0}a_{mn}\bar{a}_{mn}b_{mn}\bar{b}_{mn} + \exp(-\gamma_{1}a_{m-1n}\bar{a}_{m-1n} - \gamma_{2}b_{mn-1}\bar{b}_{mn-1} - t_{1}t_{2}\bar{a}_{m-1n}\bar{b}_{mn-1})\right]\right\}, \quad (33)$$

or in a compact form

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$$Z = (2e^{\Delta}\cosh K_1\cosh K_2)^{L^2} \int D\bar{a} Da D\bar{b} Db \exp(\mathcal{S}_{\text{Ising}} + \mathcal{S}_{\text{int}}),$$

where we have also introduced the following constants:

$$g_0 = \frac{e^{-\Delta}}{2\cosh K_1 \cosh K_2}, \qquad \gamma_i = 1 - \frac{1}{\cosh K_i} = 1 - \sqrt{1 - t_i^2}, \qquad t_i = \tanh K_i.$$
 (34)

Note that the fermionic integrals (31) and (33) are still the exact expressions for Z, even for finite lattices, provided we assume free boundary conditions both for spins and fermions. We can recognize in (33) the Ising action, which here appears as the Gaussian part of the total action [26, 27]

$$S_{\text{Ising}} = \sum_{m,n=1}^{L} a_{mn}\bar{a}_{mn} + b_{mn}\bar{b}_{mn} + a_{mn}b_{mn} + (t_1\bar{a}_{m-1n} + t_2\bar{b}_{mn-1})(a_{mn} + b_{mn}) + t_1t_2\bar{a}_{m-1n}\bar{b}_{mn-1},$$
(35)

and the non-Gaussian interaction part of the total action, which is a polynomial of degree 8 in Grassmann variables (after expanding the exponential)

$$S_{\text{int}} = g_0 \sum_{m,n=1}^{L} a_{mn} \bar{a}_{mn} b_{mn} \bar{b}_{mn} \,\mathrm{e}^{-\gamma_1 a_{m-1n} \bar{a}_{m-1n} - \gamma_2 b_{mn-1} \bar{b}_{mn-1} - t_1 t_2 \bar{a}_{m-1n} \bar{b}_{mn-1}}.$$
 (36)

The BC model differs from the Ising model by the interaction term in the action (36) which is not quadratic. Therefore the BC model is not solvable in the sense of free fermions, unlike the 2D Ising model.

It may be still of interest to recognize the structure of the phase diagram of the BC model directly from the fermionic integrals (31)–(36) before actual calculation. The interaction is introduced in the above BC integral (33) for Z with the coupling constant $g_0 \propto \exp[\beta(\Delta_0 - J_1 - J_2)]$. In the limit $\Delta \rightarrow \infty$, or $\Delta_0 \rightarrow -\infty$, which corresponds to $g_0 = 0$, the gap between the two degenerate states $S = \pm 1$ and the blockt state S = 0 becomes so large that the model reduces effectively to the 2D Ising model. For Δ_0 finite, the coupling constant g_0 is finite and the presence of the vacancy states become possible. The coupling constant g_0 increases as the number of the vacancies in a typical configuration of a system increases, with increasing Δ_0 . At zero temperature, on the other hand, as $\beta \to +\infty$, we find $g_0 = 0$ for $\Delta_0 < J_1 + J_2$, which corresponds, again, to the Ising ground state, while for $\Delta_0 > J_1 + J_2$ we gain $g_0 \to +\infty$, which means that the ground sate is empty, with vacancies only. At finite temperatures, we thus expect that there will be a line of phase transitions in the (T, Δ_0) plane, which starts from the Ising critical point at $\Delta_0 \rightarrow -\infty$, and goes lower with increasing Δ_0 , alias increasing g_0 , and terminates at $\Delta_0 = J_1 + J_2$ at zero temperature T = 0. A more sophisticated analysis of the integral (33) will be needed to define the precise form of the critical line and the existence of the tricritical point at that line with increasing dilution. In the following, for simplification in the transformations of the integrals, we will only consider the isotropic coupling case, with $K_1 = K_2 = K$, $t_1 = t_2 = t$ and $\gamma_1 = \gamma_2 = \gamma$, which corresponds to $J_1 = J_2 = J$ in the original Hamiltonian (1).

3.5. Partial bosonization

The previous action contains two pairs of Grassmann variables per site. This cannot be reduced to a one pair (minimal action) unlike for the Ising model, where half of the variables are irrelevant and can be integrated out already at lattice level without contributing to the critical behaviour. The point is that the reduced action with two variables per site readily admits QFT interpretation and simplifies the analysis in the momentum space [30, 37, 38]. In the BC case, the two pairs of fermions are coupled together by equation (36), preventing a direct integration over extra variables like a_{mn} , b_{mn} . However, as we will see in the following, it is still possible to recover the minimal Ising like action with a one pair of fermions per site using auxiliary bosonic variables. In the interaction part of the action (36), it is indeed tempting to replace the products $a_{mn}\bar{a}_{mn}$ and $b_{mn}\bar{b}_{mn}$, which are formally looking similar to occupation number operators, or local densities, by the variables

$$\eta_{mn} = a_{mn}\bar{a}_{mn}, \qquad \tau_{mn} = b_{mn}\bar{b}_{mn}, \qquad \eta_{mn}^2 = \tau_{mn}^2 = 0.$$
 (37)

This new variables η_{mn} , τ_{mn} are nilpotent (as Grassmann variables) but commuting: that is why we may abusively call them (hard core) 'bosons'. In the following, we will add also one more pair of commuting nilpotent fields $\bar{\eta}_{mn}$, $\bar{\tau}_{mn}$, to put integrals into a more symmetric form. This eventually allows us to reduce the degree of polynomials in Grassmann variables by a factor 2 each time the replacement like (37) is performed. We will see below that, in principle, we can write down an exact BC action containing a one pair of Grassmann variables and a one pair of bosonic ones per site.

To do so, we introduce the following Dirac distribution for any polynomial function f of $a_{mn}\bar{a}_{mn}$ or $b_{mn}\bar{b}_{mn}$:

$$f(a_{mn}\bar{a}_{mn}) = \int d\eta_{mn} d\bar{\eta}_{mn} f(\eta_{mn}) \exp[\bar{\eta}_{mn}(\eta_{mn} + a_{mn}\bar{a}_{mn})],$$

$$f(b_{mn}\bar{b}_{mn}) = \int d\tau_{mn} d\bar{\tau}_{mn} f(\tau_{mn}) \exp[\bar{\tau}_{mn}(\tau_{mn} + b_{mn}\bar{b}_{mn})],$$
(38)

where we assume a natural definition of the integral for commuting nilpotent variables with the following rules (similar rules are assumed for τ_{mn} , $\bar{\eta}_{mn}$ and $\bar{\tau}_{mn}$):

$$\int d\eta_{mn} 1 = 0, \qquad \int d\eta_{mn} \eta_{mn} = 1.$$
(39)

For the application of the rules like (39) in the QFT context also see [44]. Applying (38) directly in (33), we obtain the integral with the following expression for the action:

$$S = \sum_{m,n} [a_{mn}\bar{a}_{mn} + b_{mn}\bar{b}_{mn} + t^2\bar{a}_{m-1n}\bar{b}_{mn-1} + a_{mn}b_{mn} + t(\bar{a}_{m-1n} + \bar{b}_{mn-1})(a_{mn} + b_{mn}) + g_0\eta_{mn}\tau_{mn}[1 - \gamma(\eta_{m-1n} + \tau_{mn-1}) + \gamma^2\eta_{m-1n}\tau_{mn-1} - t^2\bar{a}_{m-1n}\bar{b}_{mn-1}] + \bar{\eta}_{mn}(\eta_{mn} + a_{mn}\bar{a}_{mn}) + \bar{\tau}_{mn}(\tau_{mn} + b_{mn}\bar{b}_{mn})].$$
(40)

We can now integrate over the a_{mn} 's and b_{mn} 's, and replace formally, for convenience, the variables \bar{a}_{mn} by c_{mn} and \bar{b}_{mn} by $-\bar{c}_{mn}$. We obtain:

$$S = \sum_{mn=1}^{L} \{ c_{mn} \bar{c}_{mn} (1 + \bar{\tau}_{mn}) (1 + \bar{\eta}_{mn}) + \bar{\eta}_{mn} \eta_{mn} + \bar{\tau}_{mn} \tau_{mn} + [c_{mn} (1 + \bar{\eta}_{mn}) - \bar{c}_{mn} (1 + \bar{\tau}_{mn})] t (c_{m-1n} + \bar{c}_{mn-1}) - t^2 c_{m-1n} \bar{c}_{mn-1} + g_0 \eta_{mn} \tau_{mn} [1 - \gamma (\eta_{m-1n} + \tau_{mn-1}) + \gamma^2 \eta_{m-1n} \tau_{mn-1} - t^2 c_{m-1n} \bar{c}_{mn-1}] \}.$$
(41)

The advantage is that now there are only two fermionic variables per site, which is suitable for the QFT interpretation. Note that the integral associated with the action (41) will still be the exact expression for Z. The number of the fermionic variables being reduced, the next operation is to try to integrate out, whenever possible, the auxiliary bosonic fields from action (41). In fact we can further integrate over one pair of bosonic variables, for example τ_{mn} , $\bar{\tau}_{mn}$, using the integration rules (38), since

$$\int d\tau_{mn} d\bar{\tau}_{mn} f(\tau_{mn}) \exp[\bar{\tau}_{mn}(\tau_{mn} - t(c_{m-1n} - \bar{c}_{mn-1})\bar{c}_{mn} + c_{mn}\bar{c}_{mn}(1 + \bar{\eta}_{mn}))]$$

= $f[-t(c_{m-1n} - \bar{c}_{mn-1})\bar{c}_{mn} + c_{mn}\bar{c}_{mn}(1 + \bar{\eta}_{mn})].$ (42)

There $f(\tau_{mn})$ may be any function of nilpotent variable τ_{mn} . We could also have chosen to integrate over the η_{mn} , $\bar{\eta}_{mn}$ instead. In any case, integrating over τ_{mn} , $\bar{\tau}_{mn}$ according to (42), we finally obtain the reduced integral with the local action

$$S = c_{mn}\bar{c}_{mn} + t(c_{mn} + \bar{c}_{mn})(c_{m-1n} - \bar{c}_{mn-1}) - t^2 c_{m-1n}\bar{c}_{mn-1} + \bar{\eta}_{mn}\eta_{mn} + \bar{\eta}_{mn}[\bar{c}_{mn} - t(c_{m-1n} - \bar{c}_{mn-1})]c_{mn} + g_0\eta_{mn}Q_{mn}[1 - \gamma(\eta_{m-1n} + Q_{mn-1}) + \gamma^2\eta_{m-1n}Q_{mn-1} + t^2c_{m-1n}\bar{c}_{mn-1}],$$

with

$$Q_{mn} = [c_{mn}(1 + \bar{\eta}_{mn}) - t(c_{m-1n} - \bar{c}_{mn-1})]\bar{c}_{mn}.$$
(43)

It is easy to recognize in the first line of (43) the minimal local action for the pure Ising model [30, 37] with one pair of Grassmann variables per site:

$$S_{\text{Ising}} = c_{mn}\bar{c}_{mn} + t(c_{mn} + \bar{c}_{mn})(c_{m-1n} - \bar{c}_{mn-1}) - t^2 c_{m-1n}\bar{c}_{mn-1}.$$
 (44)

This is the same action that follows by integrating a_{mn} , b_{mn} from (35). The rest of the action describes the interaction between fermions and bosons

$$S_{\text{int}} = \bar{\eta}_{mn}\eta_{mn} + \bar{\eta}_{mn}c_{mn}[\bar{c}_{mn} + t(c_{m-1n} - \bar{c}_{mn-1})] + g_0\eta_{mn}Q_{mn}[1 - \gamma(\eta_{m-1n} + Q_{mn-1}) + \gamma^2\eta_{m-1n}Q_{mn-1} + t^2c_{m-1n}\bar{c}_{mn-1}].$$
(45)

Bosonic variables can be integrated out in equations (43)–(45) only if $g_0 = 0$. In the following section, we will apply approximations in order to eliminate completely the auxiliary commuting nilpotent fields from the action, and will make use of a more symmetric form of the integration over the bosonic fields, first over $\bar{\eta}_{mn}$, $\bar{\tau}_{mn}$, then over η_{mn} , τ_{mn} .

We would like to end this section commenting the previous exact results. We finally obtained a lattice field theory with action (43) containing the same number of 'fermions' (c, \bar{c}) and 'bosons' $(\eta, \bar{\eta})$. Physically, this means that it is indeed possible to describe the system with fermionic variables for the states $S = \pm 1$ and bosonic ones for the third state S = 0. In the limit $\Delta_0 \rightarrow -\infty$, the system is completely described in terms of fermions. While with Δ_0 increasing to finite values, an interaction between fermions and bosons is added. Beyond a value Δ_{0t} , fermions form bosonic pairs: in the limit $\Delta_0 \rightarrow +\infty$, all the fermions condense into bosons, leading to a purely bosonic system. In this interpretation, the tricritical point may be seen as a particular point on the critical line where the interaction is such that an additional symmetry between fermions and bosons appears. This might correspond to super-symmetry appearing in conformal field theories describing the tricritical Ising model [17]. To our knowledge there is no evidence of super symmetry derived directly from a lattice model: the exact lattice action (43) could be a good way to see how super symmetry may emerge from a lattice model. Of course all we said so far is only speculative and needs more study to confirm or infirm this interpretation.

4. Effective action in the continuum limit

In the Ising model, the fermionic action on the lattice is quadratic and the corresponding Grassmann integral can actually be computed exactly by transformation into the momentum space for fermions. The situation for the BC model is less simple, as there is the non-Gaussian interaction part in (41), which contains terms of order up to 8th in fermions. The Grassmann integral leading to the partition function can no longer be computed directly by a simple Fourier substitution. In this sense the two-dimensional BC model is not integrable. However it is still possible to extract physical information by taking the continuous limit of the BC lattice action like (33), or (41), and analysing this limit using tools from quantum field theory.

4.1. Effective fermionic field theory

We would like to obtain an effective fermionic theory for the BC model up to order 2 in momentum k from the previous calculations, with two variables per site, in order to analyse the critical behaviour of the model. In the Ising model, the critical behaviour is given, in the continuous limit, by a mass-less theory that follows from two-variable action. In the following, we will see how to compute the mass of the BC model in its effective Gaussian part. The condition of the zero effective mass will already give the critical line in the (T, Δ_0) plane for BC. For the location of a tricritical point on that line one needs more sophisticated analysis taking into account the stability of the kinetic part of the action, which is in turn affected by the presence of the interaction. In the infrared limit, the spectrum is given by expanding the effective action, or rather the corresponding partial integral Z_k in $Z = \prod_k Z_k$, up to the second order in the momentum k. The coefficient in front of the term k^2 in the basic factor Z_k of the momentum-space spectrum for Z is the stiffness of the model. It dominates all contributions from the kinetic part of the action. For the Ising model, the stiffness is always a strictly positive coefficient. In this case, the only singularity in the spectrum then follows from the condition of vanishing mass, resulting the Ising critical point. Here in the BC model, we will show that the effective stiffness coefficient can also vanish at a special point somewhere on the line of the critical points in (T, Δ_0) plane, rendering the spectrum unstable and changing the nature of the singularity. This happens for large enough g_0 , as Δ_0 increases. We intend to identify the above singular point as an evidence for the appearance of the tricritical point, together with a segment of the first-order phase transitions at critical line at sufficiently strong dilution. In order to be able to perform the QFT analysis of the above kind, we ought to eliminate the bosonic nilpotent fields from the action, being interested in the low-momentum (small k) sector of the theory, and making reasonable approximations whenever necessary. This program also implies a more symmetric way of integration over the nilpotent fields. Instead of integrating over the variables τ_{mn} and $\bar{\tau}_{mn}$ as in equation (43), we now proceed by integrating first over $\bar{\eta}_{mn}$ and $\bar{\tau}_{mn}$ in equation (41), making use of the definition of the integral. This results the reduced integral with a new action

$$Z = (2 e^{\Delta} \cosh^2 K)^N \int \prod_{m,n} d\bar{c}_{mn} dc_{mn} d\eta_{mn} d\tau_{mn} [c_{mn}\bar{c}_{mn} + \eta_{mn}q_{mn} + \tau_{mn}\bar{q}_{mn} + \eta_{mn}\tau_{mn}]$$

$$\times \exp(\mathcal{S}_{\text{Ising}} + \mathcal{S}_{\text{int}}), \qquad (46)$$

where S_{Ising} is given in (44), while

$$S_{\text{int}} = g_0 \sum_{m,n} \eta_{mn} \tau_{mn} [(1 - \gamma \eta_{m-1n})(1 - \gamma \tau_{mn-1}) + t^2 c_{m-1n} \bar{c}_{mn-1}], \qquad (47)$$

and

$$\bar{q}_{mn} = c_{mn}\bar{c}_{mn} + tc_{mn}(c_{m-1n} - \bar{c}_{mn-1}) = c_{mn}[\bar{c}_{mn} + t(c_{m-1n} - \bar{c}_{mn-1})],$$

$$q_{mn} = c_{mn}\bar{c}_{mn} + t\bar{c}_{mn}(c_{m-1n} - \bar{c}_{mn-1}) = [c_{mn} - t(c_{m-1n} - \bar{c}_{mn-1})]\bar{c}_{mn}.$$
(48)

It is also useful to note that $q_{mn}^2 = \bar{q}_{mn}^2 = 0$, and $q_{mn}\bar{q}_{mn} = 0$. The free-fermion Ising part of the action S_{Ising} in (46) at this stage remains unchanged and is given by the standard expression (44). The above integral (46) includes as well the product of quadratic polynomial terms like $c_{mn}\bar{c}_{mn} + \eta_{mn}q_{mn} + \tau_{mn}\bar{q}_{mn} + \eta_{mn}\tau_{mn}$, which cannot be written as a block exponential. However, when integrating over the remaining variables η_{mn} and τ_{mn} , it is easy to realize that these polynomial terms *roughly* impose the following substitution rules in the action S_{int} :

$$\eta_{mn}\tau_{mn} \to c_{mn}\bar{c}_{mn}, \qquad \eta_{mn} \to \bar{q}_{mn}, \qquad \tau_{mn} \to q_{mn}. \tag{49}$$

In a sense, the above rules can be considered as an operation of approximate Dirac delta functions on the variables η_{mn} and τ_{mn} , replacing them by fermions. These rules of correspondence though are *not* exact: when expanding the exponential of S_{int} into a series, the terms will appear that couple to each other to give $c_{mn}\bar{c}_{mn}$ but not $q_{mn}\bar{q}_{mn} = 0$ as given by the above substitution rules. For example, terms such as

$$(g_0\eta_{m+1n}\tau_{m+1n}\gamma\eta_{mn}) \times (g_0\eta_{mn+1}\tau_{mn+1}\gamma\tau_{mn}), \tag{50}$$

instead of vanishing, lead to a contribution in the effective action equal to

$$g_0^2 \gamma^2 c_{mn} \bar{c}_{mn} c_{m+1n} \bar{c}_{m+1n} c_{mn+1} \bar{c}_{mn+1}.$$
(51)

Therefore there are more terms in the final effective action $S_{\text{eff}}(c_{mn}, \bar{c}_{mn})$ than in that resulting from the above substitution rules. However, we would like to apply approximations to the term with interaction, and the higher order corrections of the above kind can be neglected within this scheme anyhow. From an effective action that follows from (46), we intend to obtain the basic momentum-space factor Z_k of Z up to order 2 in momentum k, in order to study the stability of the free fermion spectrum.

In the case of the pure Ising model at criticality, the factor Z_k gives basically a $(m^2 + k^2)$ contribution to the partition function and free energy at small momenta, with mass $m^2 = 0$ at the critical point [30, 38]. In fact, there is also the stiffness coefficient λ in front of k^2 in this term, $k^2 \rightarrow \lambda k^2$. In the Ising case, this stiffness coefficient is non-singular at the critical point and can be fixed simply by its finite value at the critical temperature. In the BC case, however, we have a line of critical points as Δ_0 varies from negative to positive values. Respectively, the stiffness parameter $\lambda = \lambda(\Delta_0)$ also varies with a variation of the chemical potential Δ_0 along the critical line. The point is that in the BC case the effective stiffness coefficient vanishes at some position at the critical point of the BC model. We intend to apply an Hartree–Fock–Bogoliubov (HFB)-like approximating scheme in the momentum space in order to gain a modification of the above Ising like behaviour provided by the presence of the interaction in the BC case. This assumes a self-consistent calculation of the corrections which modify the parameters in the mass term and in the kinetic part of the action, and eventually modify the stiffness coefficient, due to the HFB decoupling of the interaction⁵.

Among the terms that contribute in Z_k to the second order in momentum are in any case those coming from the kinetic part of the free-fermion quadratic piece of the action, equation(44). In the continuous limit, with c_{m-1n} , $\bar{c}_{mn-1} \rightarrow c - \partial_x c$, $\bar{c} - \partial_y \bar{c}$, these terms are combinations of $c\partial_x c$ or $\bar{c}\partial_x c$, and $\bar{c}\partial_y \bar{c}$ or $c\partial_y \bar{c}$. From the above rules (49), we expect that the effective action will contain as well quartic contributions such as $c\bar{c}\partial_i c\partial_j \bar{c}$, with i, j = x, y, at the lowest order. This term is degree 4 in Grassmann variables and 2 in derivatives. The expansion of the exponential of such terms will give corrective coefficients to the k^2 behaviour, and may thus change the order of the transition if the renormalized stiffness vanishes. We also have to consider not only the direct substitution of the variables with the rules given above, but also the possible correction terms like (51) that contribute to the stiffness. We should also drop terms which contain a ratio of number of derivatives to the number of Grassmann variables higher strictly than 1/2 as their effect is expected to provide next-order corrections to the basic approximation scheme outlined above. After some algebra, we find the following terms that contribute to the effective action

$$S_{\text{effective}} = S_{\text{Ising}} + g_0 \sum_{m,n} c_{mn} \bar{c}_{mn} [(1 - \gamma \bar{q}_{m-1n})(1 - \gamma q_{mn-1}) + t^2 c_{m-1n} \bar{c}_{mn-1}] + g_0^2 \gamma^2 \sum_{m,n} c_{mn} \bar{c}_{mn} c_{m+1n} \bar{c}_{m+1n} c_{mn+1} \bar{c}_{mn+1} + \cdots .$$
(52)

⁵ Let us remember that the interaction terms in the BC model appear solely due to the presence of the dilute (vacancy) sites. Respectively, the strength of interaction (the coupling parameter g_0) increases with increasing rate of dilution, with variation of the chemical potential Δ_0 . The corrections with g_0 may thus appear in the mass term and the stiffness coefficients of the BC effective action within mean-field HFB analysis. In fact, as we shall see below, the relevant g_0 correction to the mass at the Gaussian (free-fermion) level already follows when we extract the effective action from (46) and (49), while the kinetic corrections, that at lattice level may be attributed to the correlations of the Ising degrees and vacancies at the same and neighbouring sites, are to be extracted self-consistently within the HFB scheme from the residual interaction in the effective action.

The above effective action defines some lattice fermionic theory with interaction. We will analyse it further on in the momentum space at low momenta, which corresponds to the continuum-limit interpretation of the model.

4.2. Continuum limit

In the continuous-limit interpretation of the above action, we replace c_{mn} by c = c(x, y)and \bar{c}_{mn} by $\bar{c} = \bar{c}(x, y)$, assuming also the substitution rules like $c_{m-1n} = c - \partial_x c$ and $c_{mn-1} = c - \partial_y c$. After a Fourier transformation of the fields, this corresponds to the low-momenta sector of the exact lattice theory around the origin $\mathbf{k} = 0$. In particular, $q_{mn} \rightarrow q = c\bar{c}(1-t) + t(\partial_x c - \partial_y \bar{c})\bar{c}$ and $\bar{q}_{mn} \rightarrow \bar{q} = c\bar{c}(1-t) - tc(\partial_x c - \partial_y \bar{c})$. The free Ising part S_{Ising} from (52) gives simply

$$S_{\text{Ising}} = \int dx \, dy [(1 - 2t - t^2)c\bar{c} - t(t+1)\bar{c}\partial_x c + t(t+1)c\partial_y\bar{c} - tc\partial_x c + t\bar{c}\partial_y\bar{c}].$$
(53)

In the above action, one can readily distinguish the mass term and the kinetic part, provided one assumes the QFT interpretation of the associated integrals⁶. Note that the next-order momentum term with product $\partial_x \partial_y$ is neglected in the above action (53) at the backbone of the first-order ∂_x , ∂_y terms⁷. In the continuous limit, the last term of the BC action (52) gives $c\bar{c}\partial_x c\partial_x \bar{c}\partial_y c\partial_y \bar{c}$, which is fourth order in derivatives and sixth degree in Grassmann variables. The ratio of these numbers is 2/3 which is higher than 1/2, and therefore this term can be discarded, as explained above. The term in factor of g_0 in (52) contains \bar{q}_{m-1n} and q_{mn-1} which need to be expanded up to the order 2 in derivatives, with $\partial_{xx}\bar{q} = 2(1-t)\partial_x c\partial_x \bar{c}$, and $\partial_{yy}q = 2(1-t)\partial_y c\partial_y \bar{c}$. The effective action finally can be written in the continuous limit as

$$\mathcal{S}_{\text{eff}} = \mathcal{S}_{\text{Ising}} + \int dx \, dy \{ g_0 c\bar{c} + g_0 c\bar{c} [t(t+2\gamma)\partial_y c\partial_x \bar{c} - \gamma(1-t)(\partial_x c\partial_x \bar{c} + \partial_y c\partial_y \bar{c})] \}.$$
(54)

In the following, we use this effective action to obtain information on the phase diagram of the BC model.

5. Spectrum analysis and phase diagram

In this section we analyse the critical properties of the effective action (54) and the low energy spectrum Z_k of Z in the momentum-space representation. In particular we develop a physical argument for the existence of a tricritical point on the phase diagram from the above fermionic action. The critical line follows already from the condition of the zero mass. At the tricritical point, we assume that the effective stiffness coefficient in factor Z_k vanishes. The Hartree–Fock–Bogoliubov (HFB)-like approximation scheme will be used to count properly the effects of the interaction [45–47].

5.1. Phase diagram

The BC model effective action of (54) includes the free-fermion Gaussian part and the quartic interaction. The quadratic part of the whole action is merely formed from S_{Ising} ,

⁶ The Ising mass is easily seen from (53) to be $m_{\text{Ising}} = 1 - 2t - t^2$, which must vanish at the critical point. Indeed, the condition of vanishing mass $1 - 2t - t^2 = 0$ gives $t_c = \sqrt{2} - 1$, alias $K_c = J/T_c = \frac{1}{2} \ln(1 + \sqrt{2})$, in agreement with the exact solution of this model on a lattice. The ordered phase corresponds to negative mass, with $t \to 1$ as $T \to 0$. The structure of the action (53) rather implies the interpretation of the pure 2D Ising model in terms of the Majorana fermions [30, 37, 38]. Respectively, one may pass to the Dirac interpretation by doubling the number of fermions in the action.

⁷ Despite that these terms with ∂_x and ∂_y are linear in momentum in the *action* they contribute as k^2 into the spectrum factor Z_k of Z, while their product may only contribute at the level of next-order corrections to Z_k , as $\underline{m} \to 0$.

but the remaining interaction term in the effective action (54) also includes quadratic term $g_0c\bar{c}$. This term, added to the Ising part of the action, will modify the original Ising mass $m_{\text{Ising}} = 1 - 2t - t^2$, and the kinetic part. The condition for the critical point in the pure Ising case is then given by $m_{\text{Ising}} = 0$ [30, 37, 38]. In the BC case, the presence of the Gaussian correction $g_0c\bar{c}$ will modify the mass term in the effective BC action: $m_{\text{Ising}} \rightarrow m_{\text{BC}} = 1 + g_0 - 2t - t^2$, which vanishes at the critical line⁸.

The approximations we intend to apply to tackle the remaining quartic part of the BC action (54) consist in replacing, in different possible ways, the two of four fermions by variational parameters, or the effective binary averages, which are then specified self-consistently from the resulting Gaussian action. This may be viewed as a kind of the HFB like approximation method, which proved to be effective in systems of quantum interacting fermions, like BCS theory of ordinary superconductivity. This also implies that calculations are to be performed rather in the momentum space than in the real space, and the corresponding symmetries are to be taken into account. The application of the HFB scheme also implies that the interaction may not be necessarily weak. From the explicit form of the quartic part of the interaction in (54), it can be seen that the decoupling of the quartic part of S_{int} produces terms which only modify the kinetic terms in the effective action, with calculations being up to order k^2 in the Z_k factor. This modification might be significant at strong dilution, rendering the appearance of the tricritical point and changing the nature of the phase transition from second to the first kind. In the next subsection, we consider in more detail the critical line of the BC model in the (T, Δ_0) plane, assuming dimensionless temperature T and chemical potential Δ_0 normalized by the exchange energy J (the isotropic case) from the BC Hamiltonian.

5.2. Critical line

The equation for the BC critical line we consider in this section is the one that follows from the condition of vanishing mass, $m_{BC} = 1 + g_0 - 2t - t^2 = 0$. In a detailed form, this equation reads

$$\tanh^{2}\left(\frac{1}{T}\right) + 2\tanh\left(\frac{1}{T}\right) - 1 = \frac{e^{\frac{\Delta_{0}}{T}}}{2\cosh^{2}\left(\frac{1}{T}\right)}.$$
(55)

This equation may be written as well in the form:

$$\sinh\left(\frac{2}{T}\right) = 1 + \frac{1}{2}e^{\frac{\Delta_0}{T}},\tag{56}$$

which in turn admits the explicit solution for Δ_0 as function of *T* in the form:

$$\Delta_0 = T \ln \left[2 \sinh \left(\frac{2}{T} \right) - 2 \right]. \tag{57}$$

This results the critical line for the BC model shown in figure 1. In the limit $\Delta_0 \rightarrow -\infty$, from either of equations (55) and (56), we recover the Ising case, with $T_c = 2.269185$. For finite Δ_0 , as vacancies are added, we obtain a slowly decreasing function for $T_c = T(\Delta_0)$, which terminates at the end point ($T_c = 0, \Delta_0 = 2$) at zero temperature, as it can be deduced from (55).

On the critical line, with zero mass, only derivative contributions remain in the action equation (54): the Ising part which gives the free fermion kinetic terms, and that which gives

⁸ The additive corrections that may contribute to the mass term from the non-Gaussian part of the action (54) are k^2 dependent and vanish as $k^2 \rightarrow 0$. They may be neglected. In the effective action (54), the principal modification of the mass term due to vacancies is realized already at the Gaussian level by the $g_0 c\bar{c}$ term, as it is commented above. The effect of the non-Gaussian part in (54) is merely that it produces corrections to the kinetic terms, after the HFB decoupling of the interaction.



Figure 1. Comparison between critical line equation (55) (plain red line) and numerical results from Monte Carlo simulations. The black filled dots are from figure 1, da Silva *et al* [9] (the Wang–Landau method). The cross symbol indicates the tricritical point identified by the same authors. The blue diamond symbols are from [10], the magenta triangles from [7], and the green squares from [6] (see also table 1 for explicit numerical values).

the residual interaction between the blockt level and the Ising doublet at the quartic level. The critical line given by (55) is plotted in figure 1, and compared with recent Monte Carlo simulations by da Silva *et al* [9, 10]. The agreement between numerical simulations and our results is very good, the mass of the system (55) being exact in that sense. The agreement is within 1% over the whole range of variation of Δ_0 on the critical line $T_c = T_c(\Delta_0)$, provided we use as input the Monte Carlo data for T_c , and evaluate theoretically Δ_0 from (57) for comparison. The numerical data for $T_c = T_c(\Delta_0)$ as a function of Δ_0 are given in table 1. Note that our results are also compatible with exact upper bond obtained by Braga *et al* [14].

5.3. Stiffness coefficient: Hartree-Fock-Bogoliubov analysis

In this section, we analyse the effect of the quartic terms in the action on the stability of the free fermion spectrum at zero mass, along the critical line $g_0 = t^2 + 2t - 1$, by considering the effect of the interaction part onto the kinetic part within the HFB-like approximating scheme [45–47]. The Ising part can be easily written in the momentum-space representation, after having defined the following transformations:

$$c(\mathbf{r}) = \frac{1}{L} \sum_{k} c_k \exp(\mathrm{i}\mathbf{k}.\mathbf{r}), \qquad \bar{c}(\mathbf{r}) = \frac{1}{L} \sum_{k} \bar{c}_k \exp(-\mathrm{i}\mathbf{k}.\mathbf{r}). \tag{58}$$

Using these transformations, the Ising part of the action gains block-diagonal form, and we find

$$S_{\text{Ising}} = \sum_{k \in S} \operatorname{it}(t+1)(k_x - k_y)(c_k \bar{c}_k - c_{-k} \bar{c}_{-k}) + 2\operatorname{it}k_x c_k c_{-k} + 2\operatorname{it}k_y \bar{c}_k \bar{c}_{-k},$$
(59)

where S is the set of Fourier modes that correspond to half of the Brillouin zone: if k is already included in S then -k is not to be included in S and vice versa, so that couples of modes

Table 1. Numerical values of the critical points $(T_c(\Delta_0), \Delta_0)$: comparison of different numerical simulations and equation (55).

	Temperature $T_c(\Delta_0)$			
Δ_0	Reference [6]	Reference [7]	Reference [10] (Wang–Landau method)	Equation (55)
-0.5		1.794(7)	1.816(2)	1.7781
0.	1.695	1.681(5)	1.714(2)	1.6740
0.5	1.567		1.584(1)	1.5427
1.0	1.398		1.413(1)	1.3695
1.5	1.150		1.155(1)	1.1162
1.87	0.800		0.800(3)	0.7712
1.9		0.764(7)	0.755(3)	0.7221
1.92	0.700		0.713(2)	0.6841
1.95	0.650		0.651(2)	0.6135
1.962	0.620		0.619(1)	0.5776
1.969	0.600		0.596(5)	0.5531
1.99	0.550		0.555(2)	0.4441
1.992	0.500		0.499(3)	0.4270

(k, -k) fill up the Brillouin zone exactly once. In fact, terms with k and -k are already combined together in (59). The mass term is dropped in (59) since we are on the critical line. The quartic term can be written in the Fourier space as

$$S_{\text{int}} = \frac{1}{L^2} \sum_{k_1 + k_2 = k_3 + k_4} V(k_2, k_4) c_{k_1} c_{k_2} \bar{c}_{k_3} \bar{c}_{k_4},$$
(60)

with the potential

$$V(\mathbf{k}_{2}, \mathbf{k}_{4}) = -\alpha k_{2}^{x} k_{4}^{y} + \alpha' (k_{2}^{x} k_{4}^{x} + k_{2}^{y} k_{4}^{y}),$$

$$\alpha = g_{0} t (t + 2\gamma), \qquad \alpha' = g_{0} \gamma (1 - t).$$
(61)

Up to now we only expressed the action in the Fourier space, or in the momentum-space representation, without further approximations. In order to see if the second-order line is stable, we use a quantum mean-field-like approximation in momentum space, similar to the HFB method. To do so, we decompose the fourth-order interacting terms into sums of quadratic terms with coefficients to be determined self-consistently. These coefficients are actually two-point correlation functions for fermions in the momentum space. The interaction can be decoupled in different ways. For example, considering the terms contributing to the Ising action, we may take account of the averages $\langle c_k \bar{c}_k \rangle$, $\langle c_{-k} \bar{c}_{-k} \rangle$, $\langle c_k c_{-k} \rangle$ and $\langle \bar{c}_k \bar{c}_{-k} \rangle$. There are also three different ways to decouple the interacting term, since c_{k_1} can be paired with either of c_{k_2} , \bar{c}_{k_3} or \bar{c}_{k_4}

$$c_{k_1}c_{k_2} = \langle c_{k_1}c_{k_2} \rangle + (c_{k_1}c_{k_2} - \langle c_{k_1}c_{k_2} \rangle) \equiv \langle c_{k_1}c_{k_2} \rangle + \delta_{c_1c_2}, \tag{62}$$

where $\delta_{c_1c_2}$ is assumed to be a small fluctuation. In this case, from equation (59), the average is nonzero only for $k_1 = -k_2 = k$ or -k, with $k \in S$. We can pair the other terms by writing the action in the coefficient $g_S = 3$ different possible ways that are compatible with the symmetries of equation (59), and by using the fermionic rules

$$S_{\text{int}} = \frac{1}{L^2 g_S} \sum_{k_1 + k_2 = k_3 + k_4} V(k_2, k_4) \Big[\big(\langle c_{k_1} c_{k_2} \rangle + \delta_{c_1 c_2} \big) \big(\langle \bar{c}_{k_3} \bar{c}_{k_4} \rangle + \delta_{\bar{c}_3 \bar{c}_4} \big) \\ - \big(\langle c_{k_1} \bar{c}_{k_3} \rangle + \delta_{c_1 \bar{c}_3} \big) \big(\langle c_{k_2} \bar{c}_{k_4} \rangle + \delta_{c_2 \bar{c}_4} \big) + \big(\langle c_{k_1} \bar{c}_{k_4} \rangle + \delta_{c_1 \bar{c}_4} \big) \big(\langle c_{k_2} \bar{c}_{k_3} \rangle + \delta_{c_2 \bar{c}_3} \big) \Big].$$
(63)

The next step is to discard terms that are proportional to the squares of fluctuations δ^2 , and keep the others. After some algebra, we obtain the mean-field quadratic operator for the interaction term as follows:

$$S_{\text{int}} = \frac{1}{L^2 g_S} \sum_{\mathbf{k}, \mathbf{k}' \in S} 4c_{\mathbf{k}} c_{-\mathbf{k}} \langle \bar{c}_{\mathbf{k}'} \bar{c}_{-\mathbf{k}'} \rangle V(\mathbf{k}, \mathbf{k}') + 4\bar{c}_{\mathbf{k}} \bar{c}_{-\mathbf{k}} \langle c_{\mathbf{k}'} c_{-\mathbf{k}'} \rangle V(\mathbf{k}', \mathbf{k}) + c_{\mathbf{k}} \bar{c}_{\mathbf{k}} (\langle c_{\mathbf{k}'} \bar{c}_{\mathbf{k}'} \rangle v(\mathbf{k}, \mathbf{k}') + \langle c_{-\mathbf{k}'} \bar{c}_{-\mathbf{k}'} \rangle v(\mathbf{k}, -\mathbf{k}')) + c_{-\mathbf{k}} \bar{c}_{-\mathbf{k}} (\langle c_{\mathbf{k}'} \bar{c}_{\mathbf{k}'} \rangle v(-\mathbf{k}, \mathbf{k}') + \langle c_{-\mathbf{k}'} \bar{c}_{-\mathbf{k}'} \rangle v(-\mathbf{k}, -\mathbf{k}')),$$
(64)

where we have defined the potential

$$v(k, k') = -V(k, k) - V(k', k') + V(k, k') + V(k', k).$$
(65)

In the above expressions, there are three different kinds of quantities that contribute to the action, for example sums like $\sum_{k} c_k \bar{c}_k$, $\sum_{k} c_k \bar{c}_k k_i$ or $\sum_{k} c_k \bar{c}_k k_i k_j$, with i, j = x, y. The first term gives a contribution to the total mass, the second one corresponds to current operators, and the third one can be thought as a dispersion energy tensor. Considering the symmetries of the Ising part, and the fact that the action should be invariant by a dilation factor at criticality, we may only take account of current operators: we can drop the first two terms in the potential v(k, k') defined in equation (65). We define therefore the following unknown parameters (i = x, y):

$$t_{i} = \frac{1}{2L^{2}} \sum_{k \in S} (\langle c_{k} \bar{c}_{k} \rangle - \langle c_{-k} \bar{c}_{-k} \rangle) k_{i},$$

$$u_{i} = \frac{i}{L^{2}} \sum_{k \in S} \langle c_{k} c_{-k} \rangle k_{i}, \qquad \bar{u}_{i} = \frac{i}{L^{2}} \sum_{k \in S} \langle \bar{c}_{k} \bar{c}_{-k} \rangle k_{i}.$$
(66)

In this case, it is easy to rewrite, from the property v(k, k') = -v(-k, k') = -v(k, -k'), the effective mean-field action (64) as

$$S_{\text{int}} = \frac{1}{g_s} \sum_{k \in S} 4i c_k c_{-k} [(\alpha \bar{u}_y - \alpha' \bar{u}_x) k_x - \alpha' \bar{u}_y k_y] + 4i \bar{c}_k \bar{c}_{-k} [-\alpha' u_x k_x + (\alpha u_x - \alpha' u_y) k_y] + 2i (c_k \bar{c}_k - c_{-k} \bar{c}_{-k}) [(\alpha t_y - 2\alpha' t_x) k_x + (\alpha t_x - 2\alpha' t_y) k_y].$$
(67)

We make the further assumption that, by symmetry invariance in the momentum space, there exists a solution satisfying $\bar{u}_y = u_x$, $\bar{u}_x = u_y$ and $t_x = -t_y$, so that

$$S_{\text{int}} = \frac{1}{g_s} \sum_{k \in S} 4ic_k c_{-k} [(\alpha u_x - \alpha' u_y)k_x - \alpha' u_x k_y] + 4i\bar{c}_k \bar{c}_{-k} [-\alpha' u_x k_x + (\alpha u_x - \alpha' u_y)k_y] - 2i(c_k \bar{c}_k - c_{-k} \bar{c}_{-k})(k_x - k_y)(\alpha + 2\alpha')t_x.$$
(68)

The total effective action (with zero mass) can finally be written as

$$S_{\text{eff}} = \sum_{k \in S} i \left[t(t+1) - \frac{2}{g_S} (\alpha + 2\alpha') t_x \right] (k_x - k_y) (c_k \bar{c}_k - c_{-k} \bar{c}_{-k}) + i \frac{4}{g_S} \left[\left(\frac{g_S}{2} t + (\alpha u_x - \alpha' u_y) \right) k_x - \alpha' u_x k_y \right] c_k c_{-k} + i \frac{4}{g_S} \left[-\alpha' u_x k_x + \left(\frac{g_S}{2} t + (\alpha u_x - \alpha' u_y) \right) k_y \right] \bar{c}_k \bar{c}_{-k},$$
(69)

or in a more compact form as

$$S_{\text{eff}} = \sum_{k \in S} ic(k_x - k_y)(c_k \bar{c}_k - c_{-k} \bar{c}_{-k}) + 2i(ak_x - bk_y)c_k c_{-k} + 2i(-bk_x + ak_y)\bar{c}_k \bar{c}_{-k}, \quad (70)$$

with the following coefficients:

$$a = t + 2\frac{\alpha u_x - \alpha' u_y}{g_s},$$

$$b = 2\alpha' \frac{u_x}{g_s},$$

$$c = t(t+1) - 2t_x \frac{\alpha + 2\alpha'}{g_s}.$$
(71)

The partition function can then be written as a product over the Fourier modes $Z = \prod_{k \in S} Z_k$, with

$$Z_k = k^2 [A + B\sin 2\theta_k], \tag{72}$$

 θ_k being the angle of the vector k, and

$$A = c^{2} - 4ab, \qquad B = -c^{2} + 2(a^{2} + b^{2}).$$
 (73)

We assume that |A| is larger than |B| on the second-order critical line, until a singular point is reached, where eventually $A^2 = B^2$. Indeed, the expression (72) is valid only if the elements $A + B \sin 2\theta_k$ are all strictly positive, which is the case only if $A^2 > B^2$. This will be checked using numerical analysis. Beyond this point, the effective action is unstable and has to be modified to incorporate further corrections. In a bosonic Φ^6 Ginzburg–Landau theory describing a first-order transition, the tricritical point is usually defined as the point where both coefficients of Φ^2 and Φ^4 terms vanish. By analogy, in the present fermionic theory, it is tempting to associate the previous singular point with the effective tricritical point.

The parameters t_x , u_x and u_y are determined self-consistently from the definition equations (66). In the continuous limit, these reduce to

$$t_{x} = \frac{c}{4\pi} \int_{0}^{\pi} d\theta \frac{1 - \sin 2\theta}{A + B \sin 2\theta} = \frac{c}{4B} \left(-1 + (A + B) \frac{\operatorname{sign}(A)}{\sqrt{A^{2} - B^{2}}} \right),$$

$$u_{x} = \frac{1}{2\pi} \int_{0}^{\pi} d\theta \frac{a \sin 2\theta - b}{A + B \sin 2\theta} = \frac{1}{2B} \left(a - (aA + bB) \frac{\operatorname{sign}(A)}{\sqrt{A^{2} - B^{2}}} \right), \quad (74)$$

$$u_{y} = \frac{1}{2\pi} \int_{0}^{\pi} d\theta \frac{a - b \sin 2\theta}{A + B \sin 2\theta} = \frac{1}{2B} \left(-b + (bA + aB) \frac{\operatorname{sign}(A)}{\sqrt{A^{2} - B^{2}}} \right).$$

Numerically, we proceed the following way: starting from *T* slightly below $T_c(-\infty)$, we solve the consistency equations for t_x , u_x and u_y with the value of Δ_0 given by the critical line (55) at that given temperature. The solutions are then plugged into the coefficients A(T) and B(T), and we plot $A(T)^2 - B(T)^2$ as a function of *T*, as shown on figure 2. We repeat the process by decreasing the temperature until we reach the point where this quantity vanishes.

By doing so we find a singular point approximately located at $(T_t^*, \Delta_{0,t}^*) \simeq$ (0.42158, 1.9926). This is close to the tricritical point T_t given by Monte Carlo simulations: $(T_t, \Delta_{0,t}) \simeq (0.610, 1.9655)$ [9], and $(T_t, \Delta_{0,t}) \simeq (0.609(3), 1.966(2))$ [10]. If we assume that T_t^* represents the tricritical point, the mean-field like treatment of the underlying field theory underestimates the fluctuations, rendering the second-order critical line more stable at lower temperature as compared to Monte Carlo results, as we approach $(T_c = 0, \Delta_0 = 2)$ along the critical line. Stronger fluctuations can be simulated by lowering the value of g_s , which increases (lowers) the value of T_t^* $(\Delta_{0,t}^*)$, respectively. Instead of $g_s = 3$, taking $g_s = 2.5$ for example leads to a $T_t^* \simeq 0.48$, closer to the Monte Carlo results. This can be achieved precisely by incorporating more diagrams in the computation of the effective free energy [46]. Also, due to the fact we are in a region near $(T_c = 0, \Delta_0 = 2)$ where the change in temperature is large compared to the change of Δ_0 (the slope is vertical at this point as is seen



Figure 2. Stiffness of the spectrum: solution of HFB self-consistent equations (74) for the coefficient $A(T)^2 - B(T)^2$ as function of *T*. The temperature where $A(T)^2 - B(T)^2 = 0$ gives the location of the singular point T_t^* .

in figure 1), it is more difficult to obtain a precise value of T_t^* within a mean-field treatment. It is however important that the BC fermionic action (54) finally predicts the existence of a special (tricritical) point at the critical line somewhere close to the termination point of that line $(T_c = 0, \Delta_0 = 2)^9$. The tricritical point is defined, within this interpretation, as the point of the destruction, or loss of stability, in the effective fermionic spectrum of the action due to the modifications introduced into the kinetic part by a sufficiently strong dilution of a system by the vacancy states, which corresponds to large enough coupling constant g_0 , as it was commented above.

6. Conclusions

In this paper, we have considered the physics of the BC model as a fermionic field theory. Using Grassmann algebra, we have shown that the model can be transformed into the quantum field theoretical language in terms of Grassmann variables. This fermionic theory for the BC model is described by an exact fermionic action with interaction on a discrete lattice. This action can be reduced, after some transformations, in the continuum limit and low energy sector, to an effective continuum field theory which includes a modified Ising action, which is quadratic in fermions, and a quartic interaction. From there we have extracted the exact mass of the model and analysed the effect of the quartic term on the stability of the free fermion spectrum in the kinetic part. The condition of the zero mass already gives the critical line of phase transition points in the (T, Δ_0) plane, which is found to be in a very good agreement with the results of Monte Carlo simulations over the whole range of variation of concentration of the non-magnetic sites governed by Δ_0 . The location of the tricritical point needs for additional analysis of the excitation spectrum of the integral factors Z_k for Z around

⁹ It may also be noted that the Monte Carlo values for $(T_t, \Delta_{0,t})$ seemingly lie practically on the theoretical curve for the critical line (55)–(57). For instance, taking as input value $T_t \simeq 0.609(3)$ [10], from (57) we find $\Delta_{0,t} \simeq 1.952$, which is sufficiently close to the M-C value $\Delta_{0,t} \simeq 1.966(2)$ from this reference [10], the deviation being probably less than 1%.

the origin in the momentum space. In particular, the stiffness of the excitation spectrum (the coefficient in front of the k^2 term in factors Z_k as we expand the dispersion relation for Z in momentum variables) vanishes at a singular point T_t^* that may be identified to the tricritical point T_1 . A Hartree–Fock–Bogoliubov analysis gives an approximate location for this point on the critical line which can be compared to the numerical results of Monte Carlo simulations. The precise location of the instability point could be achieved by taking into account further diagrams contributing to the effective free energy. In any case, we have shown the existence of a singular point on the critical line, by studying the stability of the kinetic spectrum of the action at this line, where the nature of the transition is to be changed. The main result of this paper is the possibility of studying precisely first-order transition driven systems from a fermionic point of view using Grassmann algebra. The method we have applied may be useful as well for other systems where effective field theory is presented by an action similar to that of equation (54). In essence, this is a one of the simplest form of an action with 4-fermion interaction that can be written out from a unique pair of Grassmann variables at each point of the real space. Application of the same method to other extensions of the BC Hamiltonian, such as the Blume–Emery–Griffiths model [3], is also possible. Finally, at intermediate stages, a partial bosonization of the system leads to a *mixed* representation of the model not only in term of fermions but also in term of hard core bosons, as written explicitly in the lattice action of equation (43). The representations of this kind could be useful also to look for a possible interpretation of the tricritical point in the BC model as a special point in the phase diagram where an additional hidden symmetry between fermions and bosons may appear.

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