Eur. Phys. J. B **50**, 527–539 (2006)
DOI: 10.1140/epjb/e2006-00177-x

THE EUROPEAN PHYSICAL JOURNAL B

Exact solution of the one-dimensional spin-$\frac{3}{2}$ Ising model in magnetic field

A. Avella[a] and F. Mancini

Dipartimento di Fisica "E.R. Caianiello", Unità CNISM di Salerno,
Università degli Studi di Salerno, I-84081 Baronissi (SA), Italy

Received 9 November 2005 / Received in final form 23 January 2006
Published online 17 May 2006 –

Abstract. In this paper, we study the Ising model with general spin S in presence of an external magnetic field by means of the equations of motion method and of the Green's function formalism. First, the model is shown to be isomorphic to a fermionic one constituted of $2S$ species of localized particles interacting via an intersite Coulomb interaction. Then, an exact solution is found, for any dimension, in terms of a finite, complete set of eigenoperators of the latter Hamiltonian and of the corresponding eigenenergies. This explicit knowledge makes possible writing exact expressions for the corresponding Green's function and correlation functions, which turn out to depend on a finite set of parameters to be self-consistently determined. Finally, we present an original procedure, based on algebraic constraints, to exactly fix these latter parameters in the case of dimension 1 and spin $\frac{3}{2}$. For this latter case and, just for comparison, for the cases of dimension 1 and spin $\frac{1}{2}$ [F. Mancini, Eur. Phys. J. B **45**, 497 (2005)] and spin 1 [F. Mancini, Eur. Phys. J. B **47**, 527 (2005)], relevant properties such as magnetization $\langle S \rangle$ and square magnetic moment $\langle S^2 \rangle$, susceptibility and specific heat are reported as functions of temperature and external magnetic field both for ferromagnetic and antiferromagnetic couplings. It is worth noticing the use we made of composite operators describing occupation transitions among the 3 species of localized particles and the related study of single, double and triple occupancy per site.

PACS. 05.50.+q Lattice theory and statistics – 05.30.Fk Fermion systems and electron gas – 75.10.-b General theory and models of magnetic ordering

1 Introduction

In a previous article [1], we have shown that a system constituted of q species of particles, satisfying Fermi statistics, subject to finite-range interactions and localized on the sites of a Bravais lattice, is exactly solvable in any dimension. By *exactly solvable* we mean that it is always possible finding a complete, finite set of eigenenergies and eigenoperators of the Hamiltonian which closes the hierarchy of the equations of motion. Then, formal exact expressions for the corresponding Green's functions and correlation functions can be derived. The solution is only formal as these latter turn out to depend on a finite set of parameters to be self-consistently determined. In references [2,3], we have shown how is possible to exactly fix such parameters, by means of algebraic constraints, for the one-dimensional $q = 1$ and $q = 2$ cases, respectively.

In reference [1], we have also shown that this system is isomorphic to a spin-$\frac{q}{2}$ Ising-like model in presence of an external magnetic field. According to this, the exact knowledge of a complete set of eigenoperators and eigenenergies of the system in any dimension acquires an evident relevance with respect to the hoary problem of solving the two-dimensional (in presence of an external magnetic field) and the three-dimensional Ising models. In particular, the exact knowledge of the eigenenergies of the system can shed some light on the energy scales ruling the physical properties and the magnetic response of the system and can find an application as unbiased check for the approximate solutions present in the literature. Moreover, this approach can eventually open a new route in the quest for an exact solution for these systems in higher dimensions as we have shown that it is always possible finding a formal exact expressions for the corresponding Green's functions and correlation functions. The solution is only formal as these latter turn out to depend on a finite set of parameters to be self-consistently determined. We have also shown how is possible to exactly fix such parameters, by means of algebraic constraints, for the one-dimensional case and we are now working on the possibility to use other algebraic constraints and topological relations for higher dimensions.

In this article, we apply this formulation to the one-dimensional $q = 3$ case. This model is isomorphic to the one-dimensional Ising model for spin $S = \frac{3}{2}$ in presence of an external magnetic field. This latter model can be exactly solved by means of the transfer matrix method

[a] e-mail: avella@sa.infn.it

which reduces the solution to an eigenvalue problem of the fourth order (generally, we have an eigenvalue problem of the $2S+1$th order). Unfortunately, the analytic solutions of a fourth order equation are well known, but absolutely untractable and any result, along this way, could be obtained only by means of numerical techniques, which surely do not facilitate a microscopic understanding of the properties of the system (see, for instance, Ref. [4]). In 1967, by means of a perturbation method, Suzuki, Tsujiyama and Katsura managed to reduce the order of the problem to the largest integer smaller than $S+1$ in the case of zero external magnetic field and exactly computed the energy, the specific heat and susceptibility [5]. One year later, Obokata and Oguchi [6] managed to apply the Bethe approximation, which becomes exact in one dimension, to the system and to recover the same exact results obtained by Suzuki. These latter were also recovered, few years later, by Silver and Frankel [7], who managed to formulate the problem as a difference equation of order $2S+1$ by an inductive technique and to reduce the order to the largest integer smaller than $S+1$ in the case of zero external magnetic field.

The spin-$\frac{3}{2}$ Ising model in one dimension shows magnetic plateaus [8–11], i.e. topological quantization of the magnetization at the ground state of the system due to magnetic excitations, leading to the qualitatively same structures of the magnetization profiles of the Heisenberg model. According to this, the study of this classical system can shed some light on the plateau mechanism and if it has purely quantum origin or can also depend on dimerization, frustration, single-ion anisotropy or periodic field. These plateaus have been predicted not only in theoretical study but also have been observed in experimental studies. For example, Narumi et al. [12,13] observed the magnetic plateaus in the magnetization curve for both $[Ni_2(Medpt)_2(\mu - ox)(H_2O)_2](ClO_4)_2$ $2H_2O$ and $[Ni_2(Medpt)_2(\mu - ox)(\mu\text{-}N_3)](ClO_4)_{0.5}$ H_2O. Goto et al. [14] reported the existence of the magnetization plateau at 0.25 in spin-1 3,3,5,5-tetrakis (N-tert-butylaminxyl) biphenyl (BIP-TENO). In three dimensions and with additional terms in the Hamiltonian, the spin-$\frac{3}{2}$ Ising model have been initially introduced to give a qualitative description of phase transition observed in the compound $DyVO_4$ [15] and also to describe ternary mixtures [16]. In particular, the phase diagram is not well known in contrast to the case $S=1$, which represents a special case of the Blume-Capel [17–20] and of the Blume-Emery-Griffiths [21] models often used to study a variety of interesting physical systems and, in particular, ^{3}He – ^{4}He mixtures, fluid mixtures and critical phenomena. The mean field treatment [22] predicts that the phase diagram differs for integer and half-odd-integer spins and does not present any multicritical point. While renormalization-group calculations [23,24] and Monte Carlo simulations [25] suggest the existence of a multicritical point, transfer matrix and conformal invariance studies [26] show that there is no multicritical point in the phase diagram. Unfortunately, Bethe-Peierls [27,28] and two-spin-cluster approximations [29] have not been performed in the low-temperature region. In qualitative agreement with the mean-field analysis, we can also find results from the self-consistent Ornstein-Zernike approximation [30].

In this manuscript, we present the exact solution of the model in presence of an external magnetic field. In the first section, we present the model. In the following section, we give the general solution in terms of the eigenoperators and of the eigenenergies. In the third section, we specialize the solution to the one-dimensional $q=3$–$S=\frac{3}{2}$ case. In the fourth section, we show how to close the self-consistent equations and compute all relevant correlation functions. In the fifth section, we present relevant properties such as magnetization $\langle S\rangle$ and square magnetic moment $\langle S^2\rangle$, susceptibility and specific heat as functions of the temperature and the external magnetic field both for ferromagnetic and antiferromagnetic couplings. Concluding remarks follow.

2 The model

We have analyzed a system constituted of q species of interacting particles obeying Fermi statistics, localized on the sites of a Bravais lattice and whose dynamics is ruled by the following grand-canonical Hamiltonian

$$H = -\mu \sum_{\mathbf{i},a} n_a(i) + \frac{1}{2} \sum_{\mathbf{ij},ab} V_{ab}(\mathbf{i},\mathbf{j}) n_a(i) n_b(j) \qquad (2.1)$$

where $\mathbf{i}$ stands for the lattice vector $\mathbf{R}_i$ and $i=(\mathbf{i},t)$. $n_a(i) = c_a^\dagger(i)c_a(i)$ is the particle density operator of particles of species a at the site $\mathbf{i}$. $c_a(i)$ and $c_a^\dagger(i)$ are annihilation and creation operators, respectively, of particles of species a at the site $\mathbf{i}$. They satisfy canonical anticommutation relations

$$\begin{aligned} \left\{c_a(\mathbf{i},t), c_b^\dagger(\mathbf{j},t)\right\} &= \delta_{ab}\delta_{\mathbf{ij}} \\ \{c_a(\mathbf{i},t), c_b(\mathbf{j},t)\} &= \left\{c_a^\dagger(\mathbf{i},t), c_b^\dagger(\mathbf{j},t)\right\} = 0 \end{aligned} \qquad (2.2)$$

μ is the chemical potential and $V_{ab}(\mathbf{i},\mathbf{j})$ is the strength of the interaction between particles of species a and b at distance $|\mathbf{i}-\mathbf{j}|$. We have supposed that the particles are frozen on the lattice sites as their masses are very large and/or the interactions are so strong that the kinetic energy is negligible.

In this manuscript, we have focused on the case in which the interaction $V_{ab}(\mathbf{i},\mathbf{j})$ does not depend on the particle species and is effective only between nearest-neighbor sites. That is, $V_{ab}(\mathbf{i},\mathbf{j}) = 2dV\alpha_{\mathbf{ij}}$ where d is the dimensionality of the system, $\alpha_{\mathbf{ij}}$ is the projector on the nearest-neighbor sites and V is the bare strength of the interaction. For a hyper-cubic lattice of lattice constant a we have

$$\begin{aligned} \alpha_{\mathbf{ij}} &= \frac{1}{N} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{R}_i - \mathbf{R}_j)} \alpha(\mathbf{k}) \\ \alpha(\mathbf{k}) &= \frac{1}{d} \sum_{n=1}^{d} \cos(k_n a) \end{aligned} \qquad (2.3)$$

where N is the number of sites.

Hereafter, for a generic operator $\Phi(i)$, we will use the following notation

$$\Phi^{\alpha}(\mathbf{i},t)=\sum_{\mathbf{j}}\alpha_{\mathbf{ij}}\Phi(\mathbf{j},t). \tag{2.4}$$

It is also useful to introduce the vectorial notation

$$c(i)=\begin{pmatrix} c_1(i)\\ c_2(i)\\ \vdots\\ c_q(i)\end{pmatrix}$$
$$c^{\dagger}(i)=\begin{pmatrix} c_1^{\dagger}(i)\ c_2^{\dagger}(i)\cdots\ c_q^{\dagger}(i)\end{pmatrix}. \tag{2.5}$$

and to define the total particle density

$$n(i)=\sum_a n_a(i)=\sum_a c_a^{\dagger}(i)c_a(i)=c^{\dagger}(i)c(i). \tag{2.6}$$

Then, the Hamiltonian (2.1) becomes

$$H=-\mu\sum_{\mathbf{i}}n(i)+dV\sum_{\mathbf{i}}n(i)n^{\alpha}(i). \tag{2.7}$$

Let us consider now the transformation

$$n(i)=\frac{q}{2}+S(i). \tag{2.8}$$

It is clear that

$$\begin{aligned} &n(i)=0\Leftrightarrow S(i)=-q/2\\ &n(i)=1\Leftrightarrow S(i)=1-q/2\\ &\vdots\\ &n(i)=q-1\Leftrightarrow S(i)=q/2-1\\ &n(i)=q\Leftrightarrow S(i)=q/2. \end{aligned} \tag{2.9}$$

Under the transformation (2.8), the Hamiltonian (2.7) can be cast in the form

$$H=-dJ\sum_i S(i)S^{\alpha}(i)-h\sum_i S(i)+E_0 \tag{2.10}$$

where we defined

$$\begin{aligned} J&=-dV\\ h&=\mu-qdV\\ E_0&=\frac{q}{2}\left(-\mu+\frac{q}{2}dV\right)N. \end{aligned} \tag{2.11}$$

The Hamiltonian (2.10) is just the d-dimensional spin-$\frac{q}{2}$ Ising model with nearest-neighbor interaction in presence of an external magnetic field. In this manuscript, we have chosen to use the particle notation (2.7), but the results that we have obtained are obviously valid for both the particle (2.7) and spin (2.10) systems after the transformation (2.8) and the definitions (2.11).

3 Composite operators and equations of motion

In order to apply the equations of motion method and the Green's function formalism, we need to identify a suitable operatorial basis [31,32]. It is immediate to verify that the particle density operator $n(i)$ has no time dependence

$$\mathrm{i}\frac{\partial}{\partial t}n(i)=[n(i),H]=0. \tag{3.1}$$

According to this, the operator $n(i)$, although it would have been a natural choice as component of the operatorial basis for such a system, is not suitable for this purpose. Let us introduce, instead, the following series of composite field operators

$$\psi_p(i)=c(i)[n^{\alpha}(i)]^{p-1}\qquad\qquad p=1,2,\ldots \tag{3.2}$$

whose first element is just $c(i)$. These fields satisfy the following hierarchy of equations of motion

$$\mathrm{i}\frac{\partial}{\partial t}\psi_p(i)=-\mu\psi_p(i)+2dV\psi_{p+1}(i). \tag{3.3}$$

Now, because of the anti-commutation relations (2.2), it can be shown that the operators $[n^{\alpha}(i)]^p$ satisfy the following relation

$$[n^{\alpha}(i)]^p=\sum_{m=1}^{2qd}A_m^{(p)}[n^{\alpha}(i)]^m \tag{3.4}$$

where the coefficients $A_m^{(p)}$ are rational numbers that can be easily determined after the algebra and the actual structure of the lattice (see App. A for $d=1$ and $q=3$). Then, for $p=2qd+1$, the hierarchy of equations of motion (3.3) closes as the additionally generated operator $\psi_{2qd+2}(i)=c(i)[n^{\alpha}(i)]^{2qd+1}$ can be rewritten in terms of the first $2qd+1$ elements of (3.2) through the relation (3.4).

According to this, the n-component composite field operator $\psi(i)$, defined as

$$\psi(i)=\begin{pmatrix}\psi_1(i)\\ \psi_2(i)\\ \vdots\\ \psi_n(i)\end{pmatrix}=\begin{pmatrix} c(i)\\ c(i)n^{\alpha}(i)\\ \vdots\\ c(i)[n^{\alpha}(i)]^{n-1}\end{pmatrix} \tag{3.5}$$

where $n=2qd+1$, is an eigenoperator of the Hamiltonian (2.7) as it satisfies the equation of motion

$$\mathrm{i}\frac{\partial}{\partial t}\psi(i)=[\psi(i),H]=\varepsilon\psi(i) \tag{3.6}$$

where the $n\times n$ energy matrix ε has the following expression

$$\varepsilon=\begin{pmatrix} -\mu & 2dV & 0 & \cdots & 0\\ 0 & -\mu & 2dV & \cdots & 0\\ \vdots & \vdots & \vdots & \vdots & \vdots\\ 0 & 0 & 0 & \cdots & 2dV\\ 0 & 2dVA_1^{(n)} & 2dVA_2^{(n)} & \cdots & -\mu+2dVA_{n-1}^{(n)}\end{pmatrix}. \tag{3.7}$$

The eigenvalues E_n of the energy matrix ε read as

$$E_m = -\mu + (m-1)V \qquad m = 1, 2, \ldots, n. \tag{3.8}$$

After (3.6), we can claim to have formally, but exactly, solved both Hamiltonians (2.7) and (2.10) as we have determined for them a complete set of eigenoperators and eigenvalues in any dimension d. The solution is only formal as we have still to compute all correlation functions.

Let us define the thermal retarded Green's function

$$G^R(i,j) = \left\langle R[\psi(i)\psi^\dagger(j)]\right\rangle = \theta(t_i - t_j)\langle\{\psi(i), \psi^\dagger(j)\}\rangle \tag{3.9}$$

where $\langle\cdots\rangle$ denotes the quantum-statistical average over the grand canonical ensemble. By introducing the Fourier transform

$$G^R(i,j) = \frac{\mathrm{i}}{(2\pi)^{2d+1}} \iint d\omega d\mathbf{k}\, e^{i\mathbf{k}\cdot(\mathbf{R}_i - \mathbf{R}_j) - i\omega(t_i - t_j)} G^R(\mathbf{k},\omega) \tag{3.10}$$

and by means of the equation (3.6), we obtain the equation

$$[\omega - \varepsilon] G^R(\mathbf{k},\omega) = I(\mathbf{k}) \tag{3.11}$$

where $I(\mathbf{k})$ is the Fourier transform of the normalization matrix

$$I(\mathbf{i},\mathbf{j}) = \langle\{\psi(\mathbf{i},t), \psi^\dagger(\mathbf{j},t)\}\rangle. \tag{3.12}$$

Equation (3.11) gives

$$G^R(\mathbf{k},\omega) = \sum_{m=1}^{n} \frac{\sigma^{(m)}(\mathbf{k})}{\omega - E_m + \mathrm{i}\delta}. \tag{3.13}$$

The spectral density matrices $\sigma^{(m)}(\mathbf{k})$ can be calculated by means of the formula [31]

$$\sigma^{(m)}_{ab}(\mathbf{k}) = \Omega_{am} \sum_c \Omega^{-1}_{mc} I_{cb}(\mathbf{k}) \tag{3.14}$$

where Ω is the $n \times n$ matrix whose columns are the eigenvectors of the matrix ε. The correlation functions

$$C(i,j) = \langle\psi(i)\psi^\dagger(j)\rangle \tag{3.15}$$

can be immediately calculated after (3.13) and read as

$$C(\mathbf{k},\omega) = \pi \sum_{m=1}^{n} T_m \sigma^{(m)}(\mathbf{k}) \delta(\omega - E_m) \tag{3.16}$$

where

$$T_m = 1 + \tanh\left(\frac{E_m}{2T}\right) \tag{3.17}$$

T is the temperature. By similar techniques we can calculate multi-point correlation functions as $C(i,j;l_1,l_2,\ldots,l_s) = \langle\psi(i)\psi^\dagger(j)n(l_1)n(l_2)\cdots n(l_s)\rangle$. For an example, see reference [2].

Formally, (3.13) and (3.16) constitute the exact solution of the problem under analysis. The solution is only formal as the complete knowledge of the Green's function and of the correlation functions is not fully achieved owing to unknown static correlation functions appearing in the normalization matrix $I(\mathbf{k})$ because of the complex non-canonical algebra satisfied by the field $\psi(i)$. The unknown correlators are expectation values of operators not belonging to the chosen basis $\psi(i)$ and should be self-consistently calculated in order to definitively conclude the analysis and get the complete exact solution. Unfortunately, the derivation of a set of self-consistent equations capable to determine the unknown correlators is not an easy task at all. Moreover, it depends on the particular model under analysis and, in particular, on its dimension d. In reference [1], we have developed a technique to obtain a complete exact solution in the one-dimensional case ($d = 1$) by determining the unknown correlators by means of algebraic constraints. Within this framework, we have studied the 2-state [2] ($q = 1$) and the 3-state [3] ($q = 2$) models. In this article, we consider the one-dimensional 4-state ($q = 3$) model.

4 The one-dimensional 4-state model

We now apply the general formulation given in the previous Section to an infinite homogeneous chain ($d = 1$) with $q = 3$. The derivation of the relation (3.4) for this specific case and the explicit expressions of the coefficients $A^{(p)}_m$ are given in Appendix A. Accordingly, the last row of the energy matrix ε has the following non-zero entries

$$\begin{aligned} &\varepsilon_{72} = -\frac{45}{2}V \quad \varepsilon_{73} = \frac{441}{4}V \quad \varepsilon_{74} = -203V \\ &\varepsilon_{75} = \frac{735}{4}V \quad \varepsilon_{76} = -\frac{175}{2}V \quad \varepsilon_{77} = -\mu + 21V. \end{aligned} \tag{4.1}$$

The matrix Ω has the expression

$$\Omega = \begin{pmatrix} 1 & 2^6 & 1 & (2/3)^6 & (1/2)^6 & (2/5)^6 & (1/3)^6 \\ 0 & 2^5 & 1 & (2/3)^5 & (1/2)^5 & (2/5)^5 & (1/3)^5 \\ 0 & 2^4 & 1 & (2/3)^4 & (1/2)^4 & (2/5)^4 & (1/3)^4 \\ 0 & 2^3 & 1 & (2/3)^3 & (1/2)^3 & (2/5)^3 & (1/3)^3 \\ 0 & 2^2 & 1 & (2/3)^2 & (1/2)^2 & (2/5)^2 & (1/3)^2 \\ 0 & 2 & 1 & (2/3) & (1/2) & (2/5) & (1/3) \\ 0 & 1 & 1 & 1 & 1 & 1 & 1 \end{pmatrix} \tag{4.2}$$

and the normalization matrix I reads as

$$I = \begin{pmatrix} I_{11} & I_{12} & I_{13} & I_{14} & I_{15} & I_{16} & I_{17} \\ I_{12} & I_{13} & I_{14} & I_{15} & I_{16} & I_{17} & I_{27} \\ I_{13} & I_{14} & I_{15} & I_{16} & I_{17} & I_{27} & I_{37} \\ I_{14} & I_{15} & I_{16} & I_{17} & I_{27} & I_{37} & I_{47} \\ I_{15} & I_{16} & I_{17} & I_{27} & I_{37} & I_{47} & I_{57} \\ I_{16} & I_{17} & I_{27} & I_{37} & I_{47} & I_{57} & I_{67} \\ I_{17} & I_{27} & I_{37} & I_{47} & I_{57} & I_{67} & I_{77} \end{pmatrix} \tag{4.3}$$

where

$$I_{1,p} = \kappa^{(p-1)} \tag{4.4}$$

$$I_{p,7} = \sum_{m=1}^{6} I_{1,m+1} A^{(p+5)}_m \tag{4.5}$$

$$\kappa^{(p)} = \langle[n^\alpha(i)]^p\rangle\,. \tag{4.6}$$

Then, the spectral density matrices $\sigma^{(m)}$ can be easily computed by means of equation (3.14) and the correlation functions by means of equation (3.17).

It is worth noticing that, according to the structure of the normalization matrix I [(4.3) and (4.5)], which is dictated by the relation (3.4), there exist only seven independent spectral density matrices $\sigma^{(m)}_{1,p}$ and seven independent two-point correlation functions $C_{1,p} = \langle c(i)c^\dagger(i)[n^\alpha(i)]^{p-1}\rangle$. All others can be obtained as combinations of these latter according to (3.4) and (4.5).

As regards the spectral density matrices, we have

$$\sigma^{(m)} = \Sigma_m \Gamma^{(m)} \tag{4.7}$$

where Σ_m are functions of the elements $I_{1,p}$ with $p = 1, \ldots, 7$ and $\Gamma^{(m)}$ are numerical matrices. In particular, we have the expressions

$$\begin{aligned}
\Sigma_1 &= I_{1,1} \\
&+ \frac{1}{90}(-441I_{1,2} + 812I_{1,3} - 735I_{1,4} + 350I_{1,5} - 84I_{1,6} + 8I_{1,7}) \\
\Sigma_2 &= \frac{2}{15}(90I_{1,2} - 261I_{1,3} + 290I_{1,4} - 155I_{1,5} + 40I_{1,6} - 4I_{1,7}) \\
\Sigma_3 &= \frac{1}{6}(-90I_{1,2} + 351I_{1,3} - 461I_{1,4} + 274I_{1,5} - 76I_{1,6} + 8I_{1,7}) \\
\Sigma_4 &= \frac{4}{9}(30I_{1,2} - 127I_{1,3} + 186I_{1,4} - 121I_{1,5} + 36I_{1,6} - 4I_{1,7}) \\
\Sigma_5 &= \frac{1}{6}(-45I_{1,2} + 198I_{1,3} - 307I_{1,4} + 214I_{1,5} - 68I_{1,6} + 8I_{1,7}) \\
\Sigma_6 &= \frac{2}{15}(18I_{1,2} - 81I_{1,3} + 130I_{1,4} - 95I_{1,5} + 32I_{1,6} - 4I_{1,7}) \\
\Sigma_7 &= \frac{1}{90}(-30I_{1,2} + 137I_{1,3} - 225I_{1,4} + 170I_{1,5} - 60I_{1,6} + 8I_{1,7})
\end{aligned} \tag{4.8}$$

and

$$\begin{aligned}
\Gamma^{(1)}_{1,m} &= (1\ 0\ 0\ 0\ 0\ 0\ 0) \\
\Gamma^{(2)}_{1,m} &= \left(1\ 2^{-1}\ 2^{-2}\ 2^{-3}\ 2^{-4}\ 2^{-5}\ 2^{-6}\right) \\
\Gamma^{(3)}_{1,m} &= (1\ 1\ 1\ 1\ 1\ 1\ 1) \\
\Gamma^{(4)}_{1,m} &= \left(1\ (2/3)^{-1}\ (2/3)^{-2}\ (2/3)^{-3}\ (2/3)^{-4}\ (2/3)^{-5}\ (2/3)^{-6}\right) \\
\Gamma^{(5)}_{1,m} &= \left(1\ (1/2)^{-1}\ (1/2)^{-2}\ (1/2)^{-3}\ (1/2)^{-4}\ (1/2)^{-5}\ (1/2)^{-6}\right) \\
\Gamma^{(6)}_{1,m} &= \left(1\ (2/5)^{-1}\ (2/5)^{-2}\ (2/5)^{-3}\ (2/5)^{-4}\ (2/5)^{-5}\ (2/5)^{-6}\right) \\
\Gamma^{(7)}_{1,m} &= \left(1\ (1/3)^{-1}\ (1/3)^{-2}\ (1/3)^{-3}\ (1/3)^{-4}\ (1/3)^{-5}\ (1/3)^{-6}\right)
\end{aligned} \tag{4.9}$$

As regards the two-point correlation function, we have

$$C(i,j) = \delta_{\mathbf{ij}} \frac{1}{2} \sum_{m=1}^{7} T_m \sigma^{(m)} e^{-\mathrm{i}E_m(t_i - t_j)}. \tag{4.10}$$

5 Self-consistent equations

The correlation functions $C_{1,k}$ depend, through the spectral density matrices that are functions of the entries of the normalization matrix (3.14), on the correlators $\kappa^{(p)} = \langle [n^\alpha(i)]^p \rangle$ with $p = 1, \ldots, 6$. At this stage, the correlators $\kappa^{(p)}$ are unknown as the operators $[n^\alpha(i)]^p$ do not belong to the chosen basis (3.5).

To the purpose of definitively computing the correlation functions $C_{1,k}$, let us introduce the following operators

$$\begin{aligned}
\xi_a(i) &= [1 - n(i) + D(i)]c_a(i) \\
\eta_a(i) &= [n(i) - 2D(i)]c_a(i) \\
\zeta_a(i) &= D(i)c_a(i)
\end{aligned} \tag{5.1}$$

where the double $D(i)$ and the triple $T(i)$ occupancy operators at the site $\mathbf{i}$ read as

$$\begin{aligned}
D(i) &= \sum_{\substack{a,b=1 \\ a<b}}^{3} n_a(i) n_b(i) \\
T(i) &= \prod_{a=1}^{3} n_a(i).
\end{aligned} \tag{5.2}$$

The operators $\xi_a(i)$, $\eta_a(i)$ and $\zeta_a(i)$ rule the transitions among states with different particle number at the site $\mathbf{i}$: $0 \Leftrightarrow 1$, $1 \Leftrightarrow 2$, $2 \Leftrightarrow 3$, respectively. Their complex algebra is presented in detail in Appendix B. In particular, they satisfy the following relevant relations

$$\begin{aligned}
c_a(i) &= \xi_a(i) + \eta_a(i) + \zeta_a(i) \\
\xi^\dagger_a(i)\eta_b(i) &= \xi^\dagger_a(i)\zeta_b(i) = \eta^\dagger_a(i)\zeta_b(i) = 0
\end{aligned} \tag{5.3}$$

and

$$\begin{aligned}
&\xi^\dagger_a(i)n(i) = 0 \qquad \xi^\dagger_a(i)D(i) = 0 \qquad \xi^\dagger_a(i)T(i) = 0 \\
&\eta^\dagger_a(i)n(i) = \eta^\dagger_a(i) \quad \eta^\dagger_a(i)D(i) = 0 \qquad \eta^\dagger_a(i)T(i) = 0 \\
&\zeta^\dagger_a(i)n(i) = 2\zeta^\dagger_a(i) \quad \zeta^\dagger_a(i)D(i) = \zeta^\dagger_a(i) \quad \zeta^\dagger_a(i)T(i) = 0
\end{aligned} \tag{5.4}$$

for any choice of the indices a and b.

After (5.4), it is possible to show that (see Appendix C)

$$\begin{aligned}
\xi^\dagger(i)e^{-\beta H} &= \xi^\dagger(i)e^{-\beta H_{0i}} \\
\eta^\dagger(i)e^{-\beta H} &= \eta^\dagger(i)\left\{1 + \sum_{m=1}^{6} f_m [n^\alpha(i)]^m\right\} e^{-\beta H_{0i}} \\
\zeta^\dagger(i)e^{-\beta H} &= \zeta^\dagger(i)e^{-\beta H_{0i}} \\
&\quad + \zeta^\dagger(i)\sum_{m=1}^{6}(2f_m + g_m)[n^\alpha(i)]^m e^{-\beta H_{0i}}
\end{aligned} \tag{5.5}$$

where H_{0i} is a reduced part of the Hamiltonian

$$\begin{aligned}
H_{0i} &= H - H_{Ii} \\
H_{Ii} &= 2Vn(i)n^\alpha(i).
\end{aligned} \tag{5.6}$$

We have used for $\xi(i)$, $\eta(i)$ and $\zeta(i)$ the same vectorial notation that has been used for $c(i)$ (see (2.5)). The coefficients f_m and g_m are defined in Appendix C. We will exploit the relations (5.5) in order to compute the correlation functions

$$\begin{aligned}
C^{\xi\xi}_{1,k} &= \langle \xi(i)\xi^\dagger(i)[n^\alpha(i)]^{k-1}\rangle \\
C^{\eta\eta}_{1,k} &= \langle \eta(i)\eta^\dagger(i)[n^\alpha(i)]^{k-1}\rangle \qquad k = 1, \ldots, 7 \\
C^{\zeta\zeta}_{1,k} &= \langle \zeta(i)\zeta^\dagger(i)[n^\alpha(i)]^{k-1}\rangle
\end{aligned} \tag{5.7}$$

that, after the relations (5.3), sum up to $C_{1,k} = C^{\xi\xi}_{1,k} + C^{\eta\eta}_{1,k} + C^{\zeta\zeta}_{1,k}$. By means of (5.5), we have

$$\begin{aligned}
C^{\xi\xi}_{1,k} &= \frac{\langle \xi(i)\xi^\dagger(i)[n^\alpha(i)]^{k-1}\rangle_{0i}}{\langle e^{-\beta H_{Ii}}\rangle_{0i}} \\
C^{\eta\eta}_{1,k} &= \frac{\langle \eta(i)\eta^\dagger(i)[n^\alpha(i)]^{k-1}\rangle_{0i}}{\langle e^{-\beta H_{Ii}}\rangle_{0i}} \\
&\quad + \sum_{m=1}^{6} f_m \frac{\langle \eta(i)\eta^\dagger(i)[n^\alpha(i)]^{k-1+m}\rangle_{0i}}{\langle e^{-\beta H_{Ii}}\rangle_{0i}} \\
C^{\zeta\zeta}_{1,k} &= \frac{\langle \zeta(i)\zeta^\dagger(i)[n^\alpha(i)]^{k-1}\rangle_{0i}}{\langle e^{-\beta H_{Ii}}\rangle_{0i}} \\
&\quad + \sum_{m=1}^{6} (2f_m + g_m) \frac{\langle \zeta(i)\zeta^\dagger(i)[n^\alpha(i)]^{k-1+m}\rangle_{0i}}{\langle e^{-\beta H_{Ii}}\rangle_{0i}} \qquad (5.8)
\end{aligned}$$

where for a generic operator O the notation $\langle O\rangle_{0i}$ denotes the thermal average with respect to H_{0i}

$$\langle O\rangle_{0i} = \frac{\mathrm{Tr}\{Oe^{-\beta H_{0i}}\}}{\mathrm{Tr}\{e^{-\beta H_{0i}}\}}. \qquad (5.9)$$

Now, we observe that H_{0i} describes a system where the site **i** is not connected to any other site of the chain. Then, at the site **i** the local operators enjoy a free dynamics

$$\begin{aligned}
[\xi(i), H_{0i}] &= -\mu\xi(i) \\
[\eta(i), H_{0i}] &= -\mu\eta(i) \\
[\zeta(i), H_{0i}] &= -\mu\zeta(i). \qquad (5.10)
\end{aligned}$$

By means of these equations of motion and by making use of the relations (B.8), it is possible to derive

$$\begin{aligned}
\left\langle \xi(i)\xi^\dagger(i)[n^\alpha(i)]^{k-1}\right\rangle_{0i} &= \frac{1}{(1+e^{\beta\mu})^3}\left\langle [n^\alpha(i)]^{k-1}\right\rangle_{0i} \\
\left\langle \eta(i)\eta^\dagger(i)[n^\alpha(i)]^{k-1}\right\rangle_{0i} &= \frac{2e^{\beta\mu}}{(1+e^{\beta\mu})^3}\left\langle [n^\alpha(i)]^{k-1}\right\rangle_{0i} \\
\left\langle \zeta(i)\zeta^\dagger(i)[n^\alpha(i)]^{k-1}\right\rangle_{0i} &= \frac{e^{2\beta\mu}}{(1+e^{\beta\mu})^3}\left\langle [n^\alpha(i)]^{k-1}\right\rangle_{0i} \qquad (5.11)
\end{aligned}$$

and rewrite (5.8) as

$$\begin{aligned}
C^{\xi\xi}_{1,k} &= \frac{1}{(1+e^{\beta\mu})^3}\frac{\langle [n^\alpha(i)]^{k-1}\rangle_{0i}}{\langle e^{-\beta H_{Ii}}\rangle_{0i}} \\
C^{\eta\eta}_{1,k} &= \frac{2e^{\beta\mu}}{(1+e^{\beta\mu})^3}\frac{\langle [n^\alpha(i)]^{k-1}\rangle_{0i}}{\langle e^{-\beta H_{Ii}}\rangle_{0i}} \\
&\quad + \frac{2e^{\beta\mu}}{(1+e^{\beta\mu})^3}\sum_{m=1}^{6} f_m \frac{\langle [n^\alpha(i)]^{m+k-1}\rangle_{0i}}{\langle e^{-\beta H_{Ii}}\rangle_{0i}} \\
C^{\zeta\zeta}_{1,k} &= \frac{e^{2\beta\mu}}{(1+e^{\beta\mu})^3}\frac{\langle [n^\alpha(i)]^{k-1}\rangle_{0i}}{\langle e^{-\beta H_{Ii}}\rangle_{0i}} \\
&\quad + \frac{e^{2\beta\mu}}{(1+e^{\beta\mu})^3}\sum_{m=1}^{6} (2f_m + g_m) \frac{\langle [n^\alpha(i)]^{m+k-1}\rangle_{0i}}{\langle e^{-\beta H_{Ii}}\rangle_{0i}}. \qquad (5.12)
\end{aligned}$$

Therefore, we are left with the problem of computing the functions $\langle [n^\alpha(i)]^p\rangle_{0i}$.

Now, we observe that H_{0i} describes a system where the original infinite chain is split into two disconnected infinite sub-chains (the infinite chains to the left and to the right of the site **i**) plus the site **i**. Then, in the H_{0i}-representation, correlation functions which relate sites belonging to different sub-chains and/or the site **i**, can be decoupled:

$$\langle a(j)b(l)\rangle_{0i} = \langle a(j)\rangle_{0i}\langle b(l)\rangle_{0i} \qquad (5.13)$$

when, for instance, $\mathbf{j} \leq \mathbf{i} \leq \mathbf{l}$. $a(j)$ and $b(l)$ are any functions of $n(j)$ and $n(l)$, respectively. Let us recall equations (A.7) and (A.8). By using the property (5.13), we have

$$\begin{aligned}
\langle Z_0(i)\rangle_{0i} &= 2X_1 \\
\langle Z_1(i)\rangle_{0i} &= 2X_2 + X_1^2 \\
\langle Z_2(i)\rangle_{0i} &= 2X_3 + 2X_1X_2 \\
\langle Z_3(i)\rangle_{0i} &= 2X_1X_3 + X_2^2 \\
\langle Z_4(i)\rangle_{0i} &= 2X_2X_3 \\
\langle Z_5(i)\rangle_{0i} &= X_3^2 \qquad (5.14)
\end{aligned}$$

with

$$\begin{aligned}
X_1 &= \langle n^\alpha(i)\rangle_{0i} \\
X_2 &= \langle D^\alpha(i)\rangle_{0i} \\
X_3 &= \langle T^\alpha(i)\rangle_{0i}. \qquad (5.15)
\end{aligned}$$

Therefore, we have

$$\begin{aligned}
\langle [n^\alpha(i)]^p\rangle_{0i} &= \frac{1}{2^p}\Big[2X_1 + b_1^{(p)}(2X_2 + X_1^2) \\
&+ 2b_2^{(p)}(X_3 + X_1X_2) + b_3^{(p)}(2X_1X_3 + X_2^2) \\
&+ 2b_4^{(p)}X_2X_3 + b_5^{(p)}X_3^2\Big]. \qquad (5.16)
\end{aligned}$$

The problem of computing all two-point correlation functions is thus reduced to the problem of computing just three parameters: X_1, X_2 and X_3. If we suppose the system to be homogenous, we can use the following three self-consistent equations in order to determine the unknown parameters

$$\begin{aligned}
&\langle n(i)\rangle = \langle n^\alpha(i)\rangle \Rightarrow \langle n(i)e^{-\beta H_1}\rangle_{0i} = \langle n^\alpha(i)e^{-\beta H_1}\rangle_{0i} \\
&\langle D(i)\rangle = \langle D^\alpha(i)\rangle \Rightarrow \langle D(i)e^{-\beta H_1}\rangle_{0i} = \langle D^\alpha(i)e^{-\beta H_1}\rangle_{0i} \\
&\langle T(i)\rangle = \langle T^\alpha(i)\rangle \Rightarrow \langle T(i)e^{-\beta H_1}\rangle_{0i} = \langle T^\alpha(i)e^{-\beta H_1}\rangle_{0i}. \qquad (5.17)
\end{aligned}$$

By means of equations (C.2) and (B.9), we have

$$\begin{aligned}
\left\langle n(i)e^{-\beta H_{Ii}}\right\rangle_{0i} &= B_1 + \sum_{m=1}^{6}\left[f_m(B_1 + 2B_2)\right. \\
&\left. + g_m(2B_2 + 3B_3) + h_m 3B_3\right]\left\langle [n^\alpha(i)]^m\right\rangle_{0i} \\
\left\langle n^\alpha(i)e^{-\beta H_{Ii}}\right\rangle_{0i} &= X_1 + \sum_{m=1}^{6}\left[f_m B_1 + g_m B_2\right. \\
&\left. + h_m B_3\right]\left\langle [n^\alpha(i)]^{m+1}\right\rangle_{0i} \qquad (5.18)
\end{aligned}$$

$$\langle D(i)e^{-\beta H_{Ii}}\rangle_{0i} = B_2 + \sum_{m=1}^{6}[(2B_2+3B_3)f_m +(B_2+6B_3)g_m+3B_3h_m]\langle[n^\alpha(i)]^m\rangle_{0i}$$

$$\langle D^\alpha(i)e^{-\beta H_{Ii}}\rangle_{0i} = X_2 + \sum_{m=1}^{6}[B_1f_m+B_2g_m +B_3h_m]\langle D^\alpha(i)[n^\alpha(i)]^m\rangle_{0i} \quad (5.19)$$

$$\langle T(i)e^{-\beta H_{Ii}}\rangle_{0i} = B_3\Bigg[1+\sum_{m=1}^{6}(3f_m+3g_m +h_m)\Bigg]\langle[n^\alpha(i)]^m\rangle_{0i}$$

$$\langle T^\alpha(i)e^{-\beta H_{Ii}}\rangle_{0i} = X_3 + \sum_{m=1}^{6}(B_1f_m+B_2g_m +B_3h_m)\langle T^\alpha(i)[n^\alpha(i)]^m\rangle_{0i} \quad (5.20)$$

where

$$B_1 = \langle n(i)\rangle_{0i} = \frac{3e^{\beta\mu}}{e^{\beta\mu}+1}$$
$$B_2 = \langle D(i)\rangle_{0i} = \frac{3e^{2\beta\mu}}{(e^{\beta\mu}+1)^2}$$
$$B_3 = \langle T(i)\rangle_{0i} = \frac{e^{3\beta\mu}}{(e^{\beta\mu}+1)^3}. \quad (5.21)$$

We need to calculate the averages $\langle D^\alpha(i)[n^\alpha(i)]^m\rangle_{0i}$ and $\langle T^\alpha(i)[n^\alpha(i)]^m\rangle_{0i}$. By using (A.7)

$$\langle D^\alpha(i)[n^\alpha(i)]^p\rangle_{0i} = \frac{1}{2^p}\sum_{m=0}^{5} b_m^{(p)}\langle D^\alpha(i)Z_m(i)\rangle_{0i}$$
$$\langle T^\alpha(i)[n^\alpha(i)]^p\rangle_{0i} = \frac{1}{2^p}\sum_{m=0}^{5} b_m^{(p)}\langle T^\alpha(i)\cdot Z_m(i)\rangle_{0i}. \quad (5.22)$$

By recalling the definitions (A.8) and using the property (5.13)

$$\langle D^\alpha(i)[n^\alpha(i)]^p\rangle_{0i} = \frac{1}{2^p}[2X_2+3X_3+X_1X_2 +b_1^{(p)}(X_2+6X_3+X_2^2+2X_1X_2+3X_1X_3) +b_2^{(p)}(3X_3+2X_2^2+X_1X_2+6X_1X_3+4X_2X_3) +b_3^{(p)}(3X_1X_3+X_2^2+8X_2X_3+3X_3^2) +2b_4^{(p)}(2X_2X_3+3X_3^2)+3b_5^{(p)}X_3^2\Big] \quad (5.23)$$

$$\langle T^\alpha(i)[n^\alpha(i)]^p\rangle_{0i} = \frac{1}{2^p}\Big[3X_3+X_1X_3 + b_1^{(p)}(3X_3+3X_1X_3+X_2X_3) + b_2^{(p)}(X_3+X_3^2+3X_2X_3+3X_1X_3) + b_3^{(p)}(3X_2X_3+X_1X_3+3X_3^2) + b_4^{(p)}(3X_3^2+X_2X_3)+b_5^{(p)}X_3^2\Big]. \quad (5.24)$$

Summarizing, the three parameters X_1, X_2, X_3 are determined by the coupled self-consistent equations (5.18)–(5.20), where the averages $\langle[n^\alpha(i)]^m\rangle_{0i}$, $\langle D^\alpha(i)[n^\alpha(i)]^m\rangle_{0i}$ and $\langle T^\alpha(i)[n^\alpha(i)]^m\rangle_{0i}$ are computed by means of (5.16), (5.23) and (5.24), respectively. Once we know the three parameters, we can calculate the correlation functions and all the properties. For example,

$$C_{1,k}^{\xi\xi} = \frac{1-B_1+B_2-B_3}{\langle e^{-\beta H_I}\rangle_{0i}}\langle[n^\alpha(i)]^{k-1}\rangle_{0i}$$
$$C_{1,k}^{\eta\eta} = \frac{2B_1-4B_2+6B_3}{3\langle e^{-\beta H_I}\rangle_{0i}}[\langle[n^\alpha(i)]^{k-1}\rangle_{0i} + \sum_{m=1}^{6} f_m\langle[n^\alpha(i)]^{m+k-1}\rangle_{0i}]$$
$$C_{1,k}^{\zeta\zeta} = \frac{B_2-3B_3}{3\langle e^{-\beta H_I}\rangle_{0i}}[\langle[n^\alpha(i)]^{k-1}\rangle_{0i} + \sum_{m=1}^{6}(2f_m+g_m)\langle[n^\alpha(i)]^{m+k-1}\rangle_{0i}]$$
$$C_{1,k} = C_{1,k}^{\xi\xi}+C_{1,1}^{\eta\eta}+C_{1,1}^{\zeta\zeta}$$
$$\langle n\rangle = 3-3C_{1,k}$$
$$\langle D\rangle = 3-3(C_{1,1}^{\xi\xi}+\frac{3}{2}C_{1,1}^{\zeta\zeta}+2C_{1,1}^{\eta\eta})$$
$$\langle T\rangle = 1-3(\frac{1}{3}C_{1,1}^{\xi\xi}+\frac{1}{2}C_{1,1}^{\zeta\zeta}+C_{1,1}^{\eta\eta})$$
$$\kappa^{(p)} = \frac{\langle[n^\alpha(i)]^p\rangle_{0i}}{\langle e^{-\beta H_I}\rangle_{0i}} + \sum_{m=1}^{6}(B_1f_m+B_2g_m+B_3h_m)\frac{\langle[n^\alpha(i)]^{m+p}\rangle_{0i}}{\langle e^{-\beta H_I}\rangle_{0i}} \quad (5.25)$$

$$\langle n(i)[n^\alpha(i)]^p\rangle = B_1\frac{\langle[n^\alpha(i)]^p\rangle_{0i}}{\langle e^{-\beta H_I}\rangle_{i0}} + \sum_{m=1}^{6}[(B_1+2B_2)f_m+(2B_2+3B_3)g_m +3B_3h_m]\frac{\langle[n^\alpha(i)]^{m+p}\rangle_{0i}}{\langle e^{-\beta H_I}\rangle_{0i}}. \quad (5.26)$$

The coefficients f_m, g_m and h_m are defined in Appendix C. The average $\langle e^{-\beta H_I}\rangle_{0i}$ can be computed by means of (C.2) and has the expression

$$\langle e^{-\beta H_I}\rangle_{0i} = 1+\sum_{m=1}^{6}(B_1f_m+B_2g_m+B_3h_m)\langle[n^\alpha(i)]^m\rangle_{0i}. \quad (5.27)$$

6 Results

6.1 Ferromagnetic coupling J = 1

In Figure 1, we report the magnetization per site m as a function of the magnetic field h at $J=1$, the double D and the triple T occupancies per site as functions of

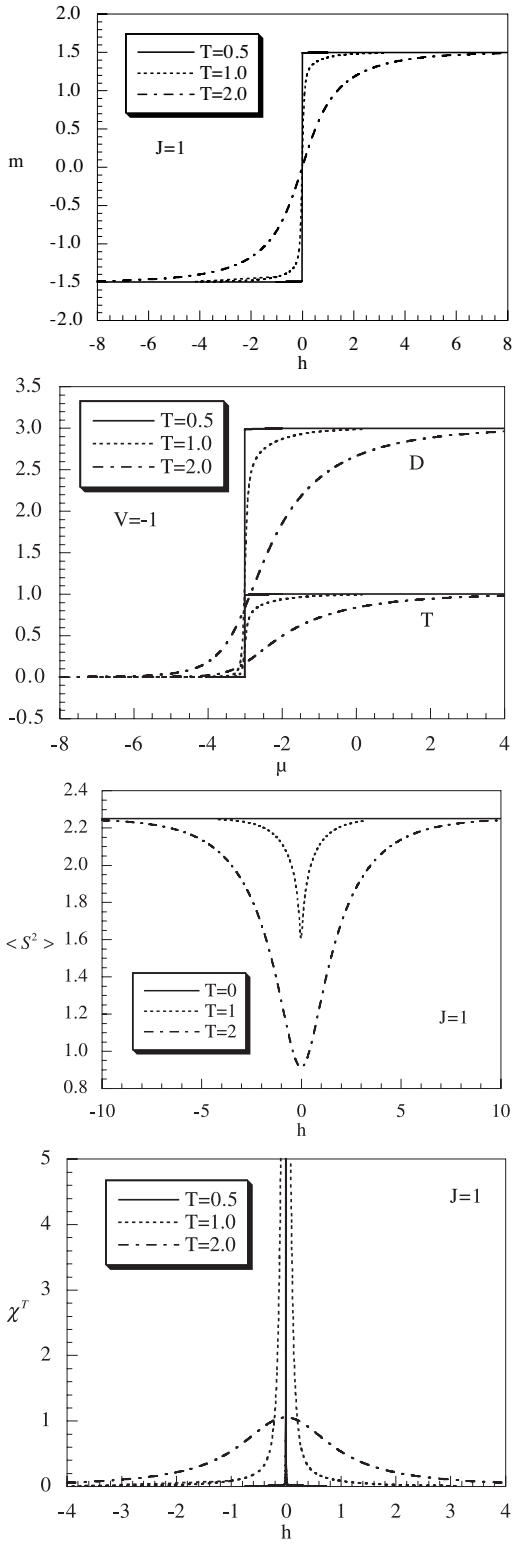

Fig. 1. (Top) Magnetization per site m as a function of the magnetic field h at $J = 1$. (Middle top) Double D and triple T occupancies per site as functions of the chemical potential μ at $V = -1$. (Middle bottom) Square magnetic moment $\langle S^2 \rangle$ per site as function of the magnetic field h at $J = 1$. (Bottom) Magnetic susceptibility χ as a function of the magnetic field h at $J = 1$. In all panels, $T = 0$ (only in middle bottom), 0.5 (except for middle bottom), 1 and 2.

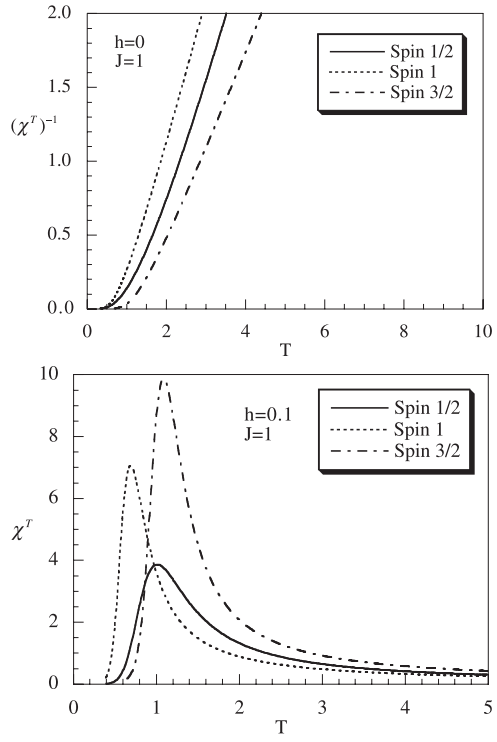

Fig. 2. (Top) Inverse magnetic susceptibility χ^{-1} at $h = 0$ and (bottom) magnetic susceptibility χ at $h = 0.1$ as functions of the temperature T at $J = 1$ and spin 1/2, 1 and 3/2.

the chemical potential μ at $V = -1$, the square magnetic moment $\langle S^2 \rangle$ per site as function of the magnetic field h at $J = 1$ and the magnetic susceptibility χ as a function of the magnetic field h at $J = 1$ and $T = 0$ (only in middle bottom panel), 0.5 (except for middle bottom panel), 1 and 2. At the lower temperature ($T = 0.5$), going from negative to positive values of the magnetic field, the magnetization jumps from $-\frac{3}{2}$ to $\frac{3}{2}$ and the susceptibility diverges exactly at zero field. This is the signature of a quite sharp transition between spin configurations with maximum possible magnetization and direction dictated by the value of the external magnetic field. This immediately reflects on the values of the double and triple occupancies that quite sharply jumps from zero to their maximum possible values: 3 and 1, respectively. The temperature just makes the transition smoother and forces the system to pass through excited states with a lower value of the absolute magnetization as it results clear by looking at the values of the square magnetic moment.

In Figure 2, we report the inverse magnetic susceptibility χ^{-1} at $h = 0$ and the magnetic susceptibility χ at $h = 0.1$ as functions of the temperature T at $J = 1$ and spin 1/2, 1 and 3/2. The sharp transition at zero temperature in zero external magnetic field is here clearly signaled by the divergence of the magnetic susceptibility for any value of the spin. At finite external magnetic field $h = 0.1$, the susceptibility presents a maximum at a finite temperature whose value depends on the value of the spin. Both at very low and very high temperatures, the magnetization stays constant at its maximum value or at zero, respectively,

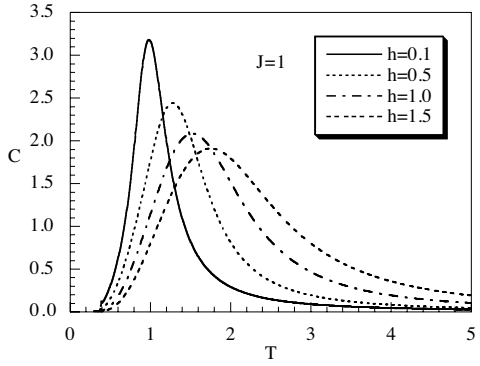

Fig. 3. Specific heat C as a function of the temperature T at $J = 1$ and $h = 0.1$, 0.5, 1 and 1.5.

almost independently on the value of the external magnetic field. According to this, in these two regimes the susceptibility is zero or practically zero. At intermediate temperatures, the value of the magnetization definitely depends on the value of the external magnetic field. This explains the bell-shape of the susceptibility curve and the presence of a maximum.

In Figure 3, we report the specific heat C as a function of the temperature T at $J = 1$ and $h = 0.1$, 0.5, 1 and 1.5. The exponential behavior at low temperatures clearly signals the presence of at least one gap in the excitation spectrum between the fully polarized state, which is the ground state for any non-zero value of the external magnetic field, and the first excited state to which corresponds a lower value of the magnetization. This behavior also explains why we have been able to see a sharp transition in the magnetization as a function of the external magnetic field at temperatures as high as $T = 0.5$. The temperature T_M, at which is clearly observable a maximum in all curves, strongly depends on the value of the external magnetic field h. In particular, T_M increases on increasing h: the gap between the ground state and the first excited state also increase on increasing h. We can speculate that $T_M \approx \frac{1}{2}(h + 2J)$, that is half of the gap existing between the fully polarized states with spin $\frac{3}{2}$ and $\frac{1}{2}$.

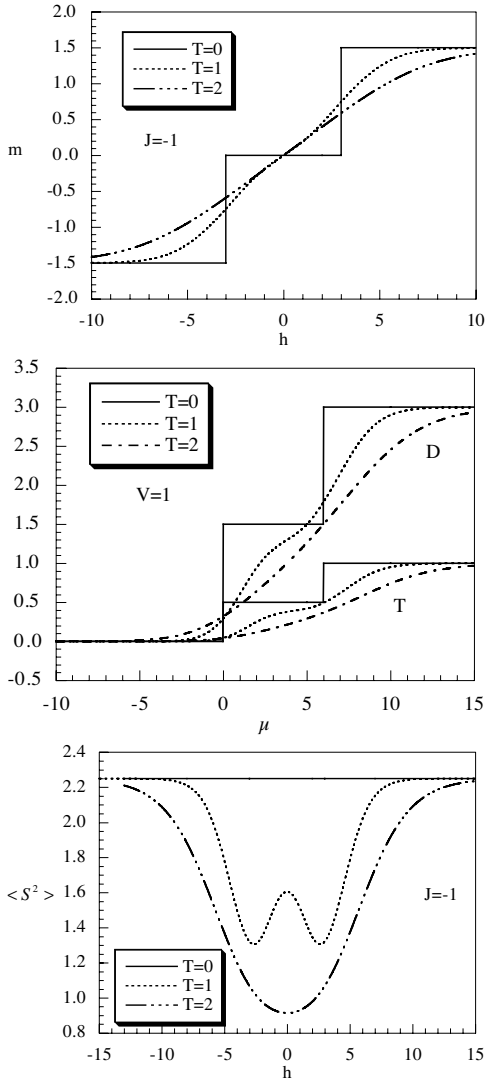

Fig. 4. (Top) Magnetization per site m as a function of the magnetic field h at $J = -1$. (Middle) Double D and triple T occupancies per site as functions of the chemical potential μ at $V = 1$. In both panels, $T = 0$, 1 and 2. (Bottom) Square magnetic moment $\langle S^2 \rangle$ per site as function of the magnetic field h at $J = -1$.

6.2 Antiferromagnetic coupling J = −1

In Figure 4, we report the magnetization per site m as a function of the magnetic field h at $J = -1$, the square magnetic moment $\langle S^2 \rangle$ per site as function of the magnetic field h at $J = -1$ and the double D and the triple T occupancies per site as functions of the chemical potential μ at $V = 1$ and $T = 0$, 1 and 2. At zero temperature, going from negative to positive values of the magnetic field, the magnetization first jumps from $-\frac{3}{2}$ to 0 at $h = 3J$ and then from 0 to $\frac{3}{2}$ at $h = -3J$. At these values of the external magnetic field, the state of lower energy changes from the fully polarized one with spin $-\frac{3}{2}$ ($E = 0$) to the antiferromagnetically aligned one with spins $\frac{3}{2}$ and $-\frac{3}{2}$ ($E = -\frac{3}{2}h + \frac{9}{2}J$) and from this latter to the the fully polarized one with spin $\frac{3}{2}$ ($E = -3h$), respectively. The double and the triple occupancies behave accordingly. The temperature just makes the transition smoother as it results clear by looking at the values of the square magnetic moment. These latter also show the typical antiferromagnetic behavior that will be easily identified in the features of the susceptibility discussed below.

In Figure 5, we report the magnetic susceptibility χ at $J = -1$ as a function of the external magnetic field h for $T = 0.8$, 1, 1.5, 2, 3 and the temperature T for $h = 0$ and spin 1/2, 1 and 3/2. As we could expect from the magnetization curves, the susceptibility diverges, at zero temperature, at the critical values discussed above and is null for all other values. On increasing the temperature, the susceptibility becomes finite for any value of the external magnetic field, although not negligible only in an

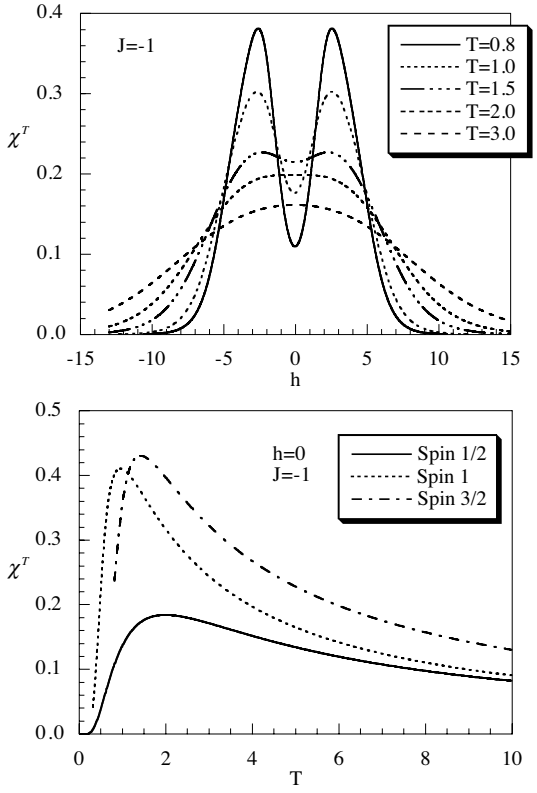

Fig. 5. Magnetic susceptibility χ at $J = -1$ as a function of (top) external magnetic field h for $T = 0.8$, 1, 1.5, 2, 3 and (bottom) temperature T for $h = 0$ and spin 1/2, 1 and 3/2.

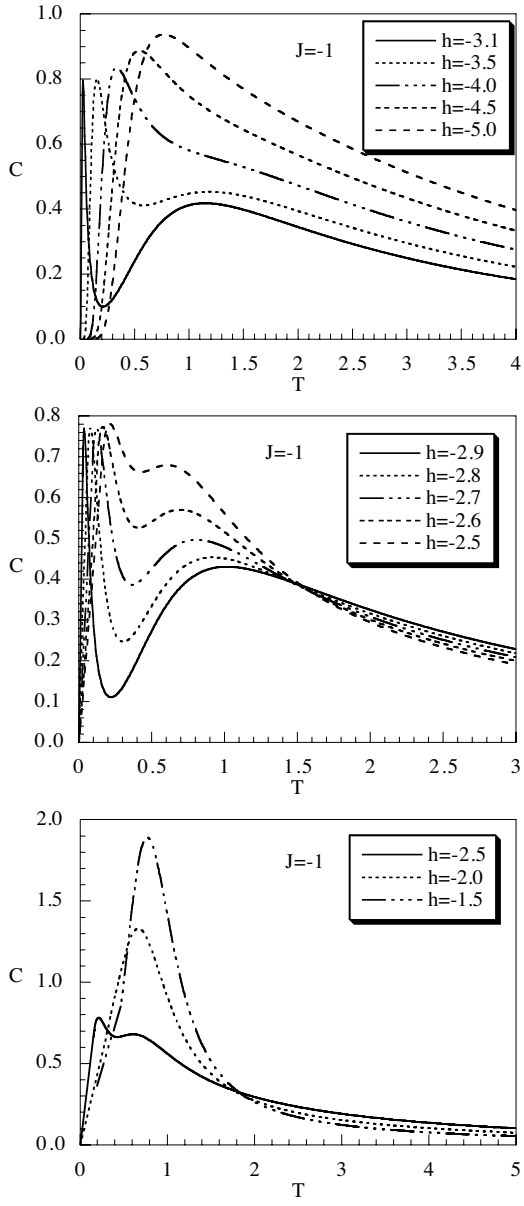

Fig. 6. Specific heat C as a function of the temperature T at $J = -1$ and $h = -5 \Rightarrow -1.5$.

increasing, but finite, range of values. According to this, as the integral of the curves over the whole axis should give a constant value, 3, that is, the larger jump in the magnetization, the heights of the two peaks steadily decrease on increasing the temperature. As a function of the temperature, the susceptibility has the typical thermal activated behavior of the parallel antiferromagnetic susceptibility for any value of the spin. According to this, we can interpret the position of the maximum as the temperature at which the system loses any memory of its antiferromagnetic ground state at zero temperature.

In Figure 6, we report the specific heat C as a function of the temperature T at $J = -1$ and $h = -5 \Rightarrow -1.5$. The curves seem to show the typical pattern caused by the interplay between at least two gaps in the excitation spectrum: $h - 3J$ and $h - 2J$. These would correspond to transitions between the fully polarized state with spin $-\frac{3}{2}$ and the antiferromagnetically aligned state with spins $\frac{3}{2}$ and $-\frac{3}{2}$ and the fully polarized state with spin $-\frac{1}{2}$, respectively. The vanishing value of the first gap, in the range of values of the external magnetic field presented in the figures, could explain the much larger sensitivity of the magnetization to temperature with respect to what happens in the ferromagnetic state. It is worth noticing the appearance of crossing points [33] for $3J < h < 2.5J$ and $2.5J < h < 1.5J$.

7 Conclusions

We have studied the Ising model with general spin S in presence of an external magnetic field by means of the equations of motion method and of the Green's function formalism. First, the model has been shown to be isomorphic to a fermionic one constituted of $2S$ species of localized particles interacting via an intersite Coulomb interaction. Then, an exact solution has been found, for any dimension, in terms of a finite, complete set of eigenoperators of the latter Hamiltonian and of the corresponding eigenenergies. This explicit knowledge has made possible writing exact expressions for the corresponding Green's function and correlation functions, which turn out to depend on a finite set of parameters to be self-consistently

determined. Finally, we have presented an original procedure, based on algebraic constraints, to exactly fix these latter parameters in the case of dimension 1 and spin $\frac{3}{2}$. For this latter case and, just for comparison, for the cases of dimension 1 and spin $\frac{1}{2}$ and spin 1, relevant properties such as magnetization $\langle S\rangle$ and square magnetic moments $\langle S^2\rangle$, susceptibility and specific heat are reported as functions of temperature and external magnetic field both for ferromagnetic and antiferromagnetic couplings. Ground state properties and relevant transitions and gaps have been studied. Crossing points in the specific heat have been identified.

Appendix A: Algebraic relations

1. Formula for $n^p(i)$

Illegal variable name.

We want to find a recurrence relation for the operator $n^p(i)$, with $p \geq 1$. At first we note that

$$\begin{aligned} & n^p(i) = (n_1+n_2+n_3)^p = \textstyle\sum_{n=0}^{p} \binom{p}{n} \\ & \times \textstyle\sum_{l=0}^{n} \binom{n}{l} n_1^{m-n} n_2^{n-l} n_3^l = [n_1^p + n_2^p + n_3^p] \\ & + \textstyle\sum_{n=1}^{p-1} \binom{p}{n} [n_1^{p-n} n_2^n + n_1^{p-n} n_3^n + n_2^{p-n} n_3^n] \\ & + \textstyle\sum_{n=2}^{p-1} \binom{p}{n} \sum_{l=1}^{n-1} \binom{n}{l} n_1^{p-n} n_2^{n-l} n_3^l \end{aligned} \tag{A.1}$$

Because of the property $n_k^p = n_k$, (A.1) takes the form

$$n^p(i) = n(i) + D(i) \sum_{n=1}^{p-1} \binom{p}{n} + T(i) \sum_{n=2}^{p-1} \binom{p}{n} \sum_{l=1}^{n-1} \binom{n}{l} \tag{A.2}$$

where $D(i)$ and $T(i)$ are the double and triple occupancy operators as defined in (5.2).

The sums in (A.2) can be analytically performed

$$\begin{aligned} & b_1^{(p)} = \textstyle\sum_{n=1}^{p-1} \binom{p}{n} = 2^p - 2 \\ & b_2^{(p)} = \textstyle\sum_{n=2}^{p-1} \binom{p}{n} \sum_{l=1}^{n-1} \binom{n}{l} = 3(1 - 2^p + 3^{p-1}) \end{aligned} \tag{A.3}$$

and we have the algebraic relation

$$n^p(i) = n(i) + b_1^{(p)} D(i) + b_2^{(p)} T(i) \tag{A.4}$$

2. Formula for $[n^\alpha(i)]^p$

By recalling that

$$[n^\alpha(i)] = \frac{1}{2}[n(i+a) + n(i-a)] \tag{A.5}$$

we have for $p = 2, 3 \cdots\cdots$

$$\begin{aligned} & [n^\alpha(i)]^p = \tfrac{1}{2^p} \textstyle\sum_{m=0}^{p} \binom{p}{m} n^{p-m}(i+a) n^m(i-a) \\ & = \tfrac{1}{2^p} n^p(i+a) + \tfrac{1}{2^p} n^p(i-a) + \tfrac{1}{2^p} \textstyle\sum_{m=1}^{p-1} \binom{p}{m} \\ & \times n^{p-m}(i+a) n^m(i-a). \end{aligned} \tag{A.6}$$

Because of the algebraic relation (A.4) we obtain

$$[n^\alpha(i)]^p = \frac{1}{2^p} \sum_{m=0}^{5} b_m^{(p)} Z_m(i) \tag{A.7}$$

where the operators $Z_m(i)$ are defined as

$$\begin{aligned} & Z_0(i) = 2n^\alpha(i) \\ & Z_1(i) = 2D^\alpha(i) + n(i+a)n(i-a) \\ & Z_2(i) = 2T^\alpha(i) + n(i+a)D(i-a) + n(i-a)D(i+a) \\ & Z_3(i) = n(i+a)T(i-a) + D(i+a) \\ & \times D(i-a) + n(i-a)T(i+a) \\ & Z_4(i) = D(i+a)T(i-a) + D(i-a)T(i+a) \\ & Z_5(i) = T(i+a)T(i-a) \end{aligned} \tag{A.8}$$

and the new coefficients $b_m^{(p)}$ have the expressions

$$\begin{aligned} & b_0^{(p)} = 1 \\ & b_3^{(p)} = \textstyle\sum_{m=1}^{p-1} \binom{p}{m} b_2^{(m)} = 4(-1 + 2^{2p-2} + 3 \cdot 2^{p-1} - 3^p) \\ & b_4^{(p)} = \textstyle\sum_{m=1}^{p-1} \binom{p}{m} b_1^{(p-m)} b_2^{(m)} = \\ & 5(1 - 2^{2p} - 2^{p+1} + 2 \cdot 3^p - 5^{p-1}) \\ & b_5^{(p)} = \textstyle\sum_{m=1}^{p-1} \binom{p}{m} b_2^{(p-m)} b_2^{(m)} = \\ & 6(-1 + 5 \cdot 2^{p-1} + 5 \cdot 2^{2p-1} - 10 \cdot 3^{p-1} - 5^p + 6^{p-1}). \end{aligned} \tag{A.9}$$

By solving (A.7) with respect to the quantities $Z_m(i)$ we obtain the recurrence relation

$$[n^\alpha(i)]^p = \sum_{m=1}^{6} A_m^{(p)} [n^\alpha(i)]^m \tag{A.10}$$

where the coefficients $A_m^{(p)}$ are rational numbers defined as

$$\begin{aligned} & A_1^{(p)} = \tfrac{1}{2^p}[2b_0^{(p)} - b_1^{(p)} + \tfrac{2}{3}b_2^{(p)} - \tfrac{1}{2}b_3^{(p)} + \tfrac{2}{5}b_4^{(p)} - \tfrac{1}{3}b_5^{(p)}] \\ & A_2^{(p)} = \tfrac{1}{2^p}[2b_1^{(p)} - 2b_2^{(p)} + \tfrac{11}{6}b_3^{(p)} - \tfrac{5}{3}b_4^{(p)} + \tfrac{137}{90}b_5^{(p)}] \\ & A_3^{(p)} = \tfrac{1}{2^p}[\tfrac{4}{3}b_2^{(p)} - 2b_3^{(p)} + \tfrac{7}{3}b_4^{(p)} - \tfrac{5}{2}b_5^{(p)}] \\ & A_4^{(p)} = \tfrac{1}{2^p}[\tfrac{2}{3}b_3^{(p)} - \tfrac{4}{3}b_4^{(p)} + \tfrac{17}{9}b_5^{(p)}] \\ & A_5^{(p)} = \tfrac{1}{2^p}[\tfrac{4}{15}b_4^{(p)} - \tfrac{2}{3}b_5^{(p)}] \\ & A_6^{(p)} = \tfrac{1}{2^p}\tfrac{4}{45}b_5^{(p)}. \end{aligned} \tag{A.11}$$

We note that

$$\begin{aligned} & \textstyle\sum_{m=1}^{6} A_m^{(p)} = 1 \\ & A_m^{(p)} = \delta_{mp} \quad (p \leq 6). \end{aligned} \tag{A.12}$$

In Table 1 we give some values of the coefficients $A_m^{(p)} (p > 6)$.

$$\{\xi(i),\xi^{\dagger}(j)\}=\delta_{\mathbf{ij}}\begin{pmatrix}(1-n_2(i))(1-n_3(i)) & -c_1(i)c_2^{\dagger}(i)(1-n_3(i)) & -c_1(i)c_3^{\dagger}(i)(1-n_2(i))\\ -c_2(i)c_1^{\dagger}(i)(1-n_3(i)) & (1-n_1(i))(1-n_3(i)) & -c_2(i)c_3^{\dagger}(i)(1-n_1(i))\\ -c_3(i)c_1^{\dagger}(i)(1-n_2(i)) & -c_3(i)c_2^{\dagger}(i)(1-n_1(i)) & (1-n_1(i))(1-n_2(i))\end{pmatrix} \tag{B.1}$$

$$\{\eta(i),\eta^{\dagger(j)}\}=\delta_{\mathbf{ij}}\begin{pmatrix}n_2(i)+n_3(i)-2n_2(i)n_3(i) & c_1(i)c_2^{\dagger}(i)(1-2n_3(i)) & c_1(i)c_3^{\dagger}(i)(1-2n_2(i))\\ c_2(i)c_1^{\dagger}(i)(1-2n_3(i)) & n_1(i)+n_3(i)-2n_1(i)n_3(i) & c_2(i)c_3^{\dagger}(i)(1-2n_1(i))\\ c_3(i)c_1^{\dagger}(i)(1-2n_2(i)) & c_3(i)c_2^{\dagger}(i)(1-2n_1(i)) & n_1(i)+n_2(i)-2n_1(i)n_2(i)\end{pmatrix} \tag{B.2}$$

Table 1.

p	$A_1^{(p)}$	$A_2^{(p)}$	$A_3^{(p)}$	$A_4^{(p)}$	$A_5^{(p)}$	$A_5^{(p)}$
7	$-\frac{45}{4}$	$\frac{441}{8}$	$-\frac{203}{2}$	$\frac{735}{8}$	$-\frac{175}{4}$	$\frac{21}{2}$
8	$-\frac{945}{8}$	$\frac{9081}{16}$	$-\frac{8085}{8}$	$\frac{13811}{16}$	$-\frac{735}{2}$	$\frac{133}{2}$
9	$-\frac{5985}{8}$	$\frac{56763}{16}$	$-\frac{98915}{16}$	$\frac{81585}{16}$	$-\frac{32739}{16}$	$\frac{1323}{4}$
10	$-\frac{59535}{16}$	$\frac{559503}{32}$	$-\frac{480375}{16}$	$\frac{774575}{32}$	$-\frac{37485}{4}$	$\frac{22827}{16}$

Appendix B: Algebra of the projection operators

On the basis of the canonical anti-commutation relations (2.2) it is straightforward to derive the algebra satisfied by the operators $\xi_a(i)$, $\eta_a(i)$, $\zeta_a(i)$ defined in (4.2). Their anti-commutation relations are

See equations (B.1) and (B.2) above.

$$\{\zeta(i),\zeta^{\dagger}(j)\}=\delta_{\mathbf{ij}}\begin{pmatrix}n_2(i)n_3(i) & c_1(i)c_2^{\dagger}(i)n_3(i) & c_1(i)c_3^{\dagger}(i)n_2(i)\\ c_2(i)c_1^{\dagger}(i)n_3(i) & n_3(i)n_1(i) & c_2(i)c_3^{\dagger}(i)n_1(i)\\ c_3(i)c_1^{\dagger}(i)n_2(i) & c_3(i)c_2^{\dagger}(i)n_1(i) & n_1(i)n_2(i)\end{pmatrix} \tag{B.3}$$

It easy to verify that

$$\{\xi(i),\xi^{\dagger}(j)\}+\{\eta(i),\eta^{\dagger}(j)\}+\{\zeta(i),\zeta^{\dagger}(j)\}=\delta_{\mathbf{ij}}\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}. \tag{B.4}$$

Other relevant algebraic properties are

$$\begin{aligned}\textstyle\sum_{a=1}^{3}\xi_a(i)\xi_a^{\dagger}(i)&=3(1-n(i)+D(i)-T(i))\\ \textstyle\sum_{a=1}^{3}\xi_a^{\dagger}(i)\xi_a(i)&=n(i)-2D(i)+3T(i)\end{aligned} \tag{B.5}$$

$$\begin{aligned}\textstyle\sum_{a=1}^{3}\eta_a(i)\eta_a^{\dagger}(i)&=2n(i)-4D(i)+6T(i)\\ \textstyle\sum_{a=1}^{3}\eta_a^{\dagger}(i)\eta_a(i)&=2D(i)-6T(i)\end{aligned} \tag{B.6}$$

$$\begin{aligned}\textstyle\sum_{a=1}^{3}\zeta_a(i)\zeta_a^{\dagger}(i)&=D(i)-3T(i)\\ \textstyle\sum_{a=1}^{3}\zeta_a^{\dagger}(i)\zeta_a(i)&=3T(i).\end{aligned} \tag{B.7}$$

By means of these relations we can express the particle density operator, the double and triple occupancy operators as

$$\begin{aligned}n(i)&=3-\textstyle\sum_{a=1}^{3}(\xi_a(i)\xi_a^{\dagger}(i)+\eta_a(i)\eta_a^{\dagger}(i)+\zeta_a(i)\zeta_a^{\dagger}(i))\\ D(i)&=3-\textstyle\sum_{a=1}^{3}(\xi_a(i)\xi_a^{\dagger}(i)+\frac{3}{2}\eta_a(i)\eta_a^{\dagger}(i)+2\zeta_a(i)\zeta_a^{\dagger}(i))\\ T(i)&=1-\textstyle\sum_{a=1}^{3}(\frac{1}{3}\xi_a(i)\xi_a^{\dagger}(i)+\frac{1}{2}\eta_a(i)\eta_a^{\dagger}(i)+\zeta_a(i)\zeta_a^{\dagger}(i))\end{aligned} \tag{B.8}$$

Also, the following relations hold

$$\begin{aligned}n^2(i)&=n(i)+2D(i) & D^2(i)&=D(i)+6T(i)\\ n(i)D(i)&=2D(i)+3T(i) & D(i)T(i)&=3T(i)\\ n(i)T(i)&=3T(i) & T^2(i)&=T(i)\end{aligned} \tag{B.9}$$

Appendix C: Calculation of $\mathbf{e^{-\beta H_{Ii}}}$

From the definition $H_{Ii}=2Vn(i)n^{\alpha}(i)$ we have

$$e^{-\beta H_{Ii}}=1+\sum_{p=1}^{\infty}\frac{1}{p!}(-1)^p(2\beta V)^p n^p(i)[n^{\alpha}(i)]^p \tag{C.1}$$

Recalling (A.4) and (A.10) we can write

$$\begin{aligned}e^{-\beta H_{Ii}}&=1+\sum_{p=1}^{\infty}\frac{1}{p!}(-1)^p(2\beta V)^p[n(i)\\ &\quad+b_1^{(p)}D(i)+b_2^{(p)}T(i)]\sum_{m=1}^{6}A_m^{(p)}[n^{\alpha}(i)]^m\\ &=1+n(i)\sum_{m=1}^{6}f_m[n^{\alpha}(i)]^m\\ &\quad+D(i)\sum_{m=1}^{6}g_m[n^{\alpha}(i)]^m\\ &\quad+T(i)\sum_{m=1}^{6}h_m[n^{\alpha}(i)]^m\end{aligned} \tag{C.2}$$

where

$$\begin{aligned}f_m&=\sum_{p=1}^{\infty}\frac{1}{p!}(-1)^p(2\beta V)^pA_m^{(p)}\\ g_m&=\sum_{p=1}^{\infty}\frac{1}{p!}(-1)^p(2\beta V)^pb_1^{(p)}A_m^{(p)}\\ h_m&=\sum_{p=1}^{\infty}\frac{1}{p!}(-1)^p(2\beta V)^pb_2^{(p)}A_m^{(p)}.\end{aligned} \tag{C.3}$$

By using the explicit expression (A.11) of the coefficients $A_m^{(p)}$, the infinite sums in (C.3) can be analytically performed. Straightforward calculations show that the parameters f_m, g_m and h_m are linear combinations of $e^{-n\beta V}$ with n ranging from 0 to 18.

References

1. F. Mancini, Europhys. Lett. **70**, 485 (2005)
2. F. Mancini, Eur. Phys. J. B **45**, 497 (2005)
3. F. Mancini, Eur. Phys. J. B **47**, 527 (2005)
4. E. Aydmer, C. Akyüz, M. Gönülol, H. Polat (2005), e-print `arXiv:cond-mat/0507177`
5. M. Suzuki, B. Tsujiyama, S. Katsura, J. Math. Phys. **8**, 124 (1967)
6. T. Obokata T. Oguchi, J. Phys. Soc. Jpn. **25**, 322 (1968)
7. H. Silver N.E. Frankel, Prog. Theor. Phys. **46**, 737 (1971)
8. X.Y. Chen, Q. Jiang, W.Z. Shen, C.G. Zhong, J. Magn. Magn. Mat. **262**, 258 (2003)
9. V.R. Ohanyan N.S. Ananikian, Phys. Lett. A **307**, 76 (2003)
10. E. Aydmer, Chin. Phys. Lett. **21**, 2289 (2004)
11. E. Aydmer, C. Akyüz (2005), Chin. Phys. Lett. (in press)
12. Y. Narumi, M. Hagiwara, R. Sato, K. Kindo, H. Nakano, M. Takahashi, Physica B **246**, 509 (1998)
13. Y. Narumi, R. Sato, K. Kindo, M. Hagiwara, J. Magn. Magn. Mat. **177**, 685 (1998), and references therein
14. T. Goto, M.I. Bartashevich, Y. Hosokoshi, K. Kato, K. Inoue, Physica B **294**, 43 (2001)
15. J. Sivardière, M. Blume, Phys. Rev. B **5**, 1126 (1972)
16. S. Krinsky D. Mukamel, Phys. Rev. B **11**, 399 (1975)
17. M. Blume, Phys. Rev. **141**, 517 (1966)
18. H. Capel, Physica **32**, 966 (1966)
19. H. Capel, Physica **33**, 295 (1967)
20. H. Capel, Physica **37**, 423 (1967)
21. M. Blume, V. Emery, R. Griffiths, Phys. Rev. A **4**, 1071 (1971)
22. J.A. Plascak, J.G. Moreira, F.C. de Sá Barreto, Phys. Lett. A **195**, 188 (1993)
23. P.M.C. de Oliveira, Europhys. Lett. **20**, 621 (1992)
24. S.M. de Oliveira, P.M.C. de Oliveira, F.C. de Sá Barreto, J. Stat. Phys. **78**, 1619 (1995)
25. F.C. de Sá Barreto, O.F. de Alcântara Bonfim, Physica A **172**, 378 (1991)
26. J.C. Xavier, F.C. Alcaraz, D.P. Lara, J.A. Plascak, Phys. Rev. B **57**, 11575 (1998)
27. T. Kaneyoshi, J.W. Tucker, M. Jascur, Physica A **186**, 495 (1992)
28. G.L. Gal, T. Kaneyoshi, A. Khater, Physica A **195**, 174 (1993)
29. M. Jurcisin, A. Bobak, M. Jascur, Physica A **224**, 684 (1996)
30. S. Grollau, Phys. Rev. B **65**, 056130 (2002)
31. F. Mancini, A. Avella, Eur. Phys. J. B **36**, 37 (2003)
32. F. Mancini, A. Avella, Adv. Phys. **53**, 537 (2004)
33. D. Vollhardt, Phys. Rev. Lett. **78**, 1307 (1997)