Physica A 391 (2012) 1087–1096

Contents lists available at SciVerse ScienceDirect

Physica A

journal homepage: www.elsevier.com/locate/physa

Callen-like method for the classical Heisenberg ferromagnet

L.S. Campana [a], A. Cavallo [b,*], L. De Cesare [b,c], U. Esposito [a], A. Naddeo [b,c]

[a] *Dipartimento di Scienze Fisiche, Università degli Studi di Napoli "Federico II", Piazzale Tecchio 80, I-80125 Napoli, Italy*

[b] *Dipartimento di Fisica "E.R. Caianiello", Università degli Studi di Salerno, via Ponte don Melillo, I-84084 Fisciano (Salerno), Italy*

[c] *CNISM, Unità di Salerno, I-84084 Fisciano (Salerno), Italy*

ARTICLE INFO

Article history:
Received 22 July 2011
Received in revised form 14 September 2011
Available online 20 October 2011

Keywords:
Classical statistical mechanics
Magnetism
Green functions

ABSTRACT

A study of the *d*-dimensional classical Heisenberg ferromagnetic model in the presence of a magnetic field is performed within the two-time Green function's framework in classical statistical physics. We extend the well known quantum Callen method to derive analytically a new formula for magnetization. Although this formula is valid for any dimensionality, we focus on one- and three- dimensional models and compare the predictions with those arising from a different expression suggested many years ago in the context of the classical spectral density method. Both frameworks give results in good agreement with the exact numerical transfer-matrix data for the one-dimensional case and with the exact high-temperature-series results for the three-dimensional one. In particular, for the ferromagnetic chain, the zero-field susceptibility results are found to be consistent with the exact analytical ones obtained by M.E. Fisher. However, the formula derived in the present paper provides more accurate predictions in a wide range of temperatures of experimental and numerical interest.

1. Introduction

Classical spin models are widely studied in statistical mechanics and play an important role in condensed matter physics but also in other disciplines, such as biology, neural networks, etc. Despite their intrinsic simplicity with respect to the quantum counterpart, classical spin models show highly nontrivial features as, for instance, a rich phase diagram and finite-temperature criticality.

Remarkably, in many relevant situations, the investigation of classical spin models allows to obtain several information for realistic magnetic materials. Indeed, they have turned out to be extremely versatile for describing a variety of relevant phenomena. This justifies the significant effort which has been devoted for optimized implementations of Monte Carlo simulations of spin models. Besides, there are several questions related to classical spin models which may further stimulate in developing new available computational resources, more efficient algorithms and powerful techniques for obtaining satisfactory answers.

Along this direction, several methods have been employed to investigate different classical spin models such as Ising, Potts models and several variants of the basic Heisenberg model.

A very efficient tool of investigation, in strict analogy of the quantum many-body techniques, is constituted by the two-time Green functions (GF) framework in classical statistical physics, as suggested by Bogoliubov and Sadovnikov [1] some decades ago and further developed and tested in Refs. [2–5].

* Corresponding author.
E-mail address: cavallo@sa.infn.it (A. Cavallo).

0378-4371/$ – see front matter
doi:10.1016/j.physa.2011.10.007

The central problem in applying this method to quantum [6] and classical [2–5,7] spin models is to find a suitable expression for magnetization in terms of the basic two-time Green function for the specific spin Hamiltonian under study.

The same problem occurs in the related quantum [8] and classical [1–5] spectral density methods (QSDM and CSDM) which have been less frequently used in literature although they appear very effective to describe the macroscopic properties of a variety of many body systems [5].

For quantum spin-1/2 Heisenberg models, exact spin operator relations allow to solve the problem directly. The case of spin-S was solved in an elegant way by Callen [9] (in the context of the two-time GF method) providing a general formula for magnetization, successfully used in many theoretical studies.

Unfortunately, for classical Heisenberg models, a similar formula is lacking in the classical two-time GF framework [1–5]. This difficulty is related to the absence of a kinematic sum rule for the z-component of the spin vector as it happens in a quantum counterpart.

Almost three decades ago [2], in the context of the CSDM [2–5], a suitable formula for magnetization was suggested for the classical isotropic Heisenberg model. However, its analytical structure was conjectured on the ground of known asymptotic results for near-polarized and paramagnetic states and not derived by means of general physical arguments. In spite of this, also in the intermediate regimes of temperature and magnetic field, this formula provided results in very good agreement with the exact numerical transfer matrix (TM) [10,11] ones for a spin chain and with the exact high-temperature-series (HTS) data of Ref. [12], for the three-dimensional model.

Quite recently [7], a study on a class of spin models based on the classical Heisenberg Hamiltonian has provided clear evidence of the effectiveness of the old formula for magnetization suggested in Ref. [2] and of the CDSM itself to describe magnetic properties in a wide range of temperatures, in surprising agreement with high resolution simulation predictions. On this grounds, the authors were also able to explain some puzzling experimental features, confirming again that this formula appears to work surprisingly well in different contexts.

In this paper we are primarily concerned with this relevant question by accounting for an extension of the quantum Callen method to derive, in the context of the classical two-time GF-framework, and, on the ground of general arguments, an expression for magnetization of the d-dimensional classical Heisenberg model, which is just the classical analogous of the famous quantum Callen formula. Remarkably, the formula here derived reproduces the asymptotic results obtained within the CSDM [2] in the near-polarized and near-zero magnetization regimes.

To test the most reliability of our formula, here we limit ourselves to calculate relevant quantities, as the spontaneous magnetization and critical temperature for $d = 3$ and other ones for $d = 1$, and to compare our predictions with those obtained in Ref. [2]. Noteworthy is that very small deviations are found in the intermediate regime corroborating the accuracy of the formula for magnetization suggested many years ago [2] and, in turn, the robustness of that found here.

The paper is organized as follows. First, in Section 2, we introduce the classical spin model and the appropriate classical Callen-like two-time Green function with the related equation of motion which are the main ingredients for next developments. Besides, we introduce, in a unified way, the Tyablikov- and Callen-like decouplings for higher order Green functions. In Section 3 we extend the quantum Callen approach to derive the general formula for magnetization valid for arbitrary dimensionality, temperature and applied magnetic field. It is easily obtained overcoming the intrinsic difficulty related to the feature that the classical analogous of the quantum spin identities used by Callen [9] does not exist. In Section 4, self-consistent equations are obtained allowing to determine the magnetization and hence other thermodynamic quantities of experimental and numerical interest. Calculations for magnetization, transverse correlation length and critical temperature for $d > 2$ and different lattice structure are presented in Section 5. Finally, in Section 6, some conclusions are drawn.

2. The model and Callen-like Green function

The classical Heisenberg ferromagnet is described by the Hamiltonian

$$\begin{aligned}\mathcal{H} &= -\frac{1}{2}\sum_{i,j=1}^{N} J_{ij}\mathbf{S}_i\cdot\mathbf{S}_j - h\sum_{i=1}^{N} S_i^z \\ &= -\frac{1}{2}\sum_{i,j=1}^{N} J_{ij}\left(S_i^+S_j^- + S_i^zS_j^z\right) - h\sum_{i=1}^{N} S_i^z. \end{aligned} \tag{1}$$

Here N is the number of sites on a d-dimensional lattice with unitary spacing, $\left\{\mathbf{S}_j \equiv \left(S_j^x, S_j^y, S_j^z\right); i = 1, 2, \ldots, N\right\}$ are classical spin vectors with $\left|\mathbf{S}_j\right| = S$, $S_j^{\pm} = S_j^x \pm iS_j^y$, $J_{ij} = J_{ji}$, ($J_{ii} = 0$) is the spin–spin coupling and h is the applied magnetic field. Of course, the identity $\mathbf{S}_j^2 = \left(S_j^z\right)^2 + S_j^+S_j^- = S^2$ is valid. For formal simplicity, in the next developments we will assume $S = 1$. This assumption is perfectly legal in the classical context.

The model (1) can be appropriately described in terms of the $2N$ canonical variables $\phi \equiv \left\{\phi_j\right\}$ and $S^z \equiv \left\{S_j^z\right\}$, where ϕ_j is the angle between the projection of the spin vector $\mathbf{S}_j$ in the x–y-plane and the x-axis.