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EXACT THERMOSTATIC RESULTS FOR THE n-VECTOR MODEL ON THE HARMONIC CHAIN

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In this paper we report exact results on thermostatic properties of the classical n-vector model on the harmonic chain. This system is characterized by the Hamiltonian

$$H := H_0(\{p\},\{q\}) + H_1(\{q\},\{\mathbf{S}\}) \tag{1}$$

where

$$H_0(\{p\},\{q\}) := \frac{1}{2m}\sum_{j=1}^{N+1} p_j^2 + \frac{m}{2}\omega_0^2 \sum_{j=1}^{N}(q_j - q_{j+1})^2\,, \tag{2}$$

$$H_1(\{q\},\{\mathbf{S}\}) := -\sum_{j=1}^{N} W(\ell + q_{j+1} - q_j)\mathbf{S}_j \cdot \mathbf{S}_{j+1}\,. \tag{3}$$

Here H_0 is the Hamiltonian for the nearest-neighbor coupled harmonic chain which consists of a one-dimensional lattice $\ell\mathbb{Z}$ with lattice constant $\ell > 0$ and a set of $N+1$ point particles of mass $m > 0$ distributed along the Euclidean line $\mathbb{R}$ at positions $j\ell + q_j$, $j = 1, 2, \ldots, N+1$. The momentum of the jth particle is denoted by p_j and the spring constant of this chain is $m\omega_0^2$. We assume now that each particle carries a set of internal rotational degrees of freedom which we collectively represent by a classical spin, that is, by an n-component Euclidean unit vector $\mathbf{S}_j \in \mathbb{R}^n$. The Hamiltonian H_1 then models the simplest rotational invariant interaction between the spins of two nearest neighbored particles. The interaction strength between two spins is described by the real-valued even function $W : x \mapsto W(x)$ and depends on the actual interparticle distance as indicated in (3). In accordance with the harmonic approximation it is sufficient to consider only the first two terms in a

Taylor expansion of W,

$$W(\ell + q_{j+1} - q_j) \approx J + (q_{j+1} - q_j)\eta\,, \tag{4}$$

where $J := W(\ell)$ and $\eta := W'(\ell)$.

Within this approximation it is possible to decouple the vibrational and rotational degrees of freedom by introducing shifted particle positions (cf. Refs. 1 and 2 for $n = 1$)

$$x_1 := q_1\,, \quad x_j := q_j - \frac{\eta}{m\omega_0^2} \sum_{r=1}^{j-1} \mathbf{S}_r \cdot \mathbf{S}_{r+1}\,, \quad j = 2, 3, \ldots, N+1\,. \tag{5}$$

The result can be cast into the form

$$H \approx H_0(\{p\}, \{x\}) + H_{\mathrm{spin}}(\{\mathbf{S}\}) \tag{6}$$

where we have introduced the pure spin–chain Hamiltonian

$$H_{\mathrm{spin}}(\{\mathbf{S}\}) := -\sum_{j=1}^{N} \left(J\mathbf{S}_j \cdot \mathbf{S}_{j+1} + K(\mathbf{S}_j \cdot \mathbf{S}_{j+1})^2\right) \tag{7}$$

with $K := \eta^2/(2m\omega_0^2)$. Since the thermal properties of the harmonic chain are well known (see, for example, Ref. 3), we will consider only those of H_{spin}.

Special cases of the Hamiltonian (7) have already been discussed in the literature. For $K = 0$ it corresponds to Stanley's n-vector model in one dimension.[4,5] For $J = 0$ and $n \in \{2, 3\}$ a discussion is due to Vuillermot and Romerio.[6] As for the Ising case ($n = 1$), we remark that the biquadratic term in (7) lowers the specific free energy of the Ising chain simply by the constant K. However, even for $n = 1$ this term is responsible for magnetostrictive effects of the full system (6), as discussed by Mattis and Schultz.[1,2] As an aside we mention that exactly known[7] ground-state properties of the quantum version of (7) for $n = 3$, $\hat{\mathbf{S}}_j^2 = 2\hbar^2\hat{\mathbf{1}}$, $J < 0$ and $K/|J| = -1/3$ are discussed[7] in relation with Haldane's conjecture.

The basic thermostatic properties of the classical spin-chain Hamiltonian (7) can be obtained from the free energy per spin in the macroscopic limit $N \to \infty$:

$$F(\beta) := -\frac{1}{\beta} \lim_{N\to\infty} \frac{1}{N+1} \ln Z(\beta)\,, \tag{8}$$

where the canonical partition function at temperature $1/\beta k$ (k: Boltzmann's constant) for the finite chain and $n \geq 2$ may be defined by the $(N+1)(n-1)$-dimensional integral

$$Z(\beta) := \int d\mathbf{S}_1 \cdots \int d\mathbf{S}_{N+1} \exp\{-\beta H_{\mathrm{spin}}(\{\mathbf{S}\})\}\,. \tag{9}$$

For convenience we are using open boundary conditions. Furthermore, each of the above $d\mathbf{S}$ stands for the usual surface measure on the $(n-1)$-dimensional unit sphere in $\mathbb{R}^n$. We assume this measure to be normalized in the sense that $\int d\mathbf{S} = 1$ and recall its invariance under rotations

$$\int d\mathbf{S}\, f(\mathbf{S}) = \int d\mathbf{S}\, f(g\mathbf{S}). \tag{10}$$

This relation is valid for any integrable complex-valued function f and all orthogonal $n \times n$ matrices $g \in SO(n)$. Of course, for $n = 1$ the integration $\int d\mathbf{S}$ stands for the summation $\frac{1}{2}\sum_{S=\pm 1}$.

For the evaluation of the partition function (9) we note that the Hamiltonian (7) can be rewritten as $H_{\text{spin}}(\{\mathbf{S}\}) = \sum_{j=1}^{N} V(\mathbf{S}_j,\, \mathbf{S}_{j+1})$ where we have introduced the spin-pair interaction energy

$$V(\mathbf{S},\, \mathbf{S}') := -J\mathbf{S}\cdot\mathbf{S}' - K(\mathbf{S}\cdot\mathbf{S}')^2\,, \tag{11}$$

which is $SO(n)$-invariant and exchange-invariant:

$$V(g\mathbf{S},\, g\mathbf{S}') = V(\mathbf{S},\, \mathbf{S}') = V(\mathbf{S}',\, \mathbf{S})\,, \quad \text{for all } g \in SO(n). \tag{12}$$

These properties can be used to rewrite the Hamiltonian (7) as $H_{\text{spin}}(\{\mathbf{S}\}) = \sum_{j=1}^{N} V(\mathbf{S}_0,\, g_j\mathbf{S}_{j+1})$ where $\mathbf{S}_0$ is an arbitrary but fixed unit vector and the $n \times n$ matrices g_j are defined by $g_j\mathbf{S}_j := \mathbf{S}_0$. With the rotational invariance (10) the partition function (9) can be reduced to a single $d\mathbf{S}$-integration according to

$$Z(\beta) = \int d\mathbf{S}_1 \int d\mathbf{S}_2\, e^{-\beta V(\mathbf{S}_0,\mathbf{S}_2)} \cdots \int d\mathbf{S}_{N+1}\, e^{-\beta V(\mathbf{S}_0,\mathbf{S}_{N+1})} = \lambda^N(\beta) \tag{13}$$

where

$$\lambda(\beta) := \int d\mathbf{S}\, \exp\{-\beta V(\mathbf{S}_0,\, \mathbf{S})\}. \tag{14}$$

Hence, the specific free energy (8) is given by

$$F(\beta) = -(1/\beta)\ln\lambda(\beta). \tag{15}$$

What remains to be done is the integration (14). Choosing as the fixed vector $\mathbf{S}_0$ the unit vector pointing towards the northpole, $\mathbf{S}_0 = (0,\, \ldots,\, 0,\, 1)$, the function $V(\mathbf{S}_0,\, \mathbf{S})$, and therefore also $\exp\{-\beta V(\mathbf{S}_0,\, \mathbf{S})\}$, depends only on the polar angle θ if $\mathbf{S}$ is parameterized in the usual (hyper-) spherical polar coordinates, because then $\mathbf{S}_0 \cdot \mathbf{S} = \cos\theta$. Hence, the expression (14) can immediately be reduced to the following one-dimensional integral ($t := \cos\theta$):

$$\lambda(\beta) = \frac{\Gamma(n/2)}{\sqrt{\pi}\,\Gamma(\frac{n-1}{2})} \int_{-1}^{+1} dt\, e^{\beta(Jt+Kt^2)}(1-t^2)^{\frac{n-3}{2}}. \tag{16}$$

For $K = 0$ this integral can be expressed in terms of modified Bessel functions

$$\lambda(\beta) = \Gamma(n/2)\left(\frac{2}{\beta J}\right)^{\frac{n-2}{2}} I_{\frac{n-2}{2}}(\beta J)\,, \tag{17}$$

the well-known result for Stanley's n-vector chain.[4] For $K \neq 0$ an expansion in powers of βJ allows for an integration in terms of the confluent hypergeometric function[8]:

$$\lambda(\beta) = \sum_{r=0}^{\infty} \frac{\Gamma(n/2)\,(\beta J/2)^{2r}}{\Gamma(n/2+r)\,\Gamma(r+1)}\, {}_1F_1\left(r+\tfrac{1}{2};\, r+\tfrac{n}{2};\, \beta K\right) . \tag{18}$$

This series can be summed[9] in terms of a generalized hypergeometric function of two variables[10,11]:

$$\lambda(\beta) = \exp\left\{-\frac{\beta J^2}{4K}\right\} \Psi_2\left(\frac{1}{2};\frac{n}{2},\frac{1}{2};\beta K,\frac{\beta J^2}{4K}\right) . \tag{19}$$

Unfortunately, not much is known about this generalized hypergeometric function. However, for the cases $n = 1$, 2 and 3, we can express $\lambda(\beta)$ somewhat more explicitly as follows:

$$\begin{aligned}
\lambda(\beta) &= \mathrm{e}^{\beta K}\cosh(\beta J)\,, && \text{for } n=1\,,\\
\lambda(\beta) &= \frac{e^{\beta K}}{\sqrt{\pi}}\sum_{r=0}^{\infty}\frac{\Gamma\left(r+\frac{1}{2}\right)}{\Gamma(r+1)}\left(-\frac{2K}{|J|}\right)^{r} I_r(\beta|J|)\,, && \text{for } n=2\,,\\
\lambda(\beta) &= \frac{1}{2}\mathrm{e}^{-\beta J^2/4K}\left[\left(1+\frac{J}{2K}\right)\, {}_1F_1\left(\frac{1}{2};\frac{3}{2};\beta K\left(1+\frac{J}{2K}\right)^2\right)\right.\\
&\quad \left. + \left(1-\frac{J}{2K}\right)\, {}_1F_1\left(\frac{1}{2};\frac{3}{2};\beta K\left(1-\frac{J}{2K}\right)^2\right)\right], && \text{for } n=3\,.
\end{aligned} \tag{20}$$

For $n = 1$ we have used formula 7.2.4.91 of Ref. 10 leading to the expected result. For $n = 2$, in essence, we have expanded the integral (16) in powers of βK. For $n = 3$ the integral (16) obviously is reducible to the sum of two error functions with complex argument, which in turn can be expressed in terms of confluent hypergeometric functions. Equations (19) and (20) in combination with (15) summarize the main results we wish to report here. Appropriate derivatives of $\lambda(\beta)$ with respect to β lead to the basic thermostatic quantities. For example, the specific heat $c(\beta)$ is given as

$$c(\beta) = -k\beta^2 \frac{\partial^2}{\partial\beta^2}(\beta F(\beta)) = k\beta^2\left[\frac{\lambda''(\beta)}{\lambda(\beta)} - \left(\frac{\lambda'(\beta)}{\lambda(\beta)}\right)^2\right] . \tag{21}$$

Figure 1 displays this function for $n = 3$ as a surface over the $1/\beta|J|$-$K/|J|$-plane. We note that its zero-temperature value $c(\infty) = k$ is in agreement with the classical

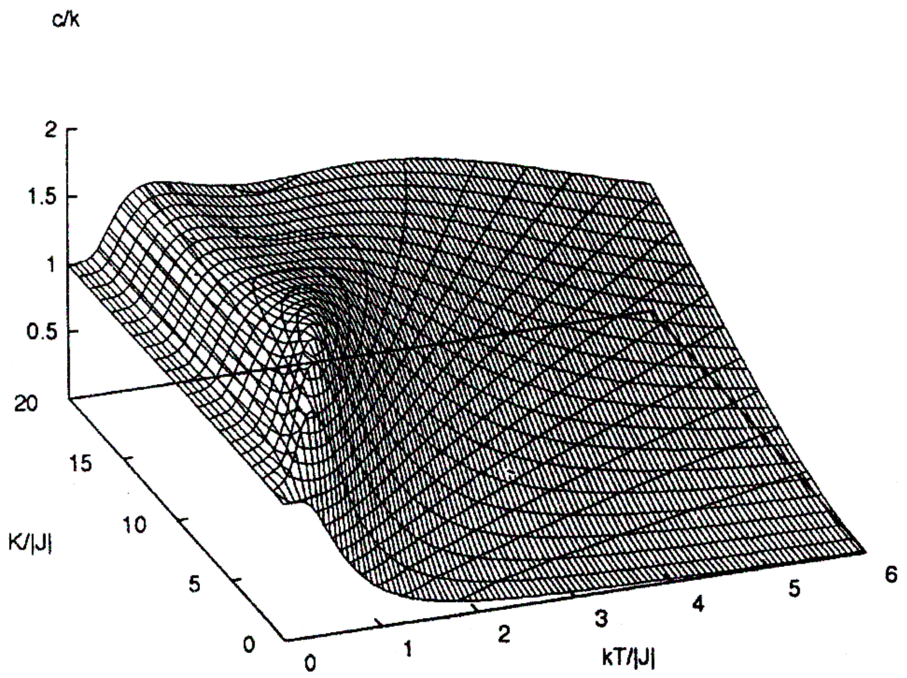

Fig. 1. The specific heat (21) for $n = 3$ as a function of the dimensionless temperature $kT/|J| := 1/\beta|J|$ and the parameter $K/|J|$.

equipartition theorem. For low temperatures and $K > 0$ the specific heat $c(\beta)$ increases linearly:

$$\frac{c(\beta)}{k} = 1 + \frac{K}{(K + |J|/2)^2\beta} + \cdots . \tag{22}$$

For high temperatures it vanishes as the inverse square of the temperature:

$$\frac{c(\beta)}{k} = \left(J^2 + \frac{4}{15}\,K^2\right)\frac{\beta^2}{3} + \cdots . \tag{23}$$

For $0 < K/|J| \lesssim 14$ the specific heat attains a maximum value in the temperature range $0 < 1/\beta|J| \lesssim 0.9$. This maximum splits for $K/|J| \gtrsim 15$ into two maxima. The global maximum of $c(\beta)$ remains near $1/\beta|J| \lesssim 1$ for large K values.

Finally, we remark that from the free energy (15) in combination with (16) or (19) one can obtain[12] further interesting properties of the system (6). Examples are the two-spin correlation function

$$\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle = \left(-\frac{\partial}{\partial J}\,F(\beta)\right)^{|i-j|}, \tag{24}$$

here $\langle\cdot\rangle$ denotes the canonical equilibrium expectation value with respect to Hamiltonian (6), the zero-field susceptibility

$$\chi_0(\beta) := \beta\left(1 + 2\sum_{r=1}^{\infty}\langle\mathbf{S}_j\cdot\mathbf{S}_{j+r}\rangle\right) = \beta\,\frac{1 - \dfrac{\partial}{\partial J}F(\beta)}{1 + \dfrac{\partial}{\partial J}F(\beta)}\,, \qquad (25)$$

and the mean lattice constant

$$a(\beta) := \ell + \langle q_{j+1} - q_j\rangle = \ell - \frac{\eta}{m\omega_0^2}\frac{\partial}{\partial J}F(\beta)\,. \qquad (26)$$

A more detailed discussion (including applications and further thermostatic properties) of the system characterized by the Hamiltonian (6) will be given elsewhere.[12]

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