PHYSICAL REVIEW E VOLUME 61, NUMBER 4 APRIL 2000

# Dynamical temperature for spin systems

Wira Bahari Nurdin* and Klaus-Dieter Schotte†
*Institut für Theoretische Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany*

(Received 13 September 1999)

A transcription of Rugh's geometrical approach to temperature is given for classical Heisenberg spin systems. For the simple case of a paramagnet with small and large numbers of spins we verify the approach. A numerical check for long spin chains using spin dynamics shows its practicality.

PACS number(s): 05.50.+q, 75.10.Hk, 75.40.Mg

## I. INTRODUCTION

Starting from a microcanonical ensemble the entropy $S$ is a function of energy. It is defined as the logarithm of the number of different states $W$ that a physical system has with a given energy $E$, that is, $S=\ln W$ with Boltzmann's constant set to unity. For a classical system with Hamilton function $\mathcal{H}$, this number is proportional to the surface of constant energy in the phase space of canonical coordinates $(q_i,p_i)$. More precisely, it is the number of points between infinitesimal neighboring surfaces given by the formula [1,2]

$$W=\int \delta(E-\mathcal{H})\prod_{i=1}^{N} dq_i\,dp_i=\int_{\mathcal{H}=E}\frac{do}{|\vec{\nabla}\mathcal{H}|}=\int_{\mathcal{H}=E}\frac{d\vec{o}\cdot\vec{\nabla}\mathcal{H}}{|\vec{\nabla}\mathcal{H}|^2} \tag{1}$$

written in the form of a Gaussian surface integral. The direction of the infinitesimal surface element $d\vec{o}$ normal to the surface of constant energy coincides with the direction of the gradient $\vec{\nabla}\mathcal{H}$. This quantity cannot in general be calculated directly for a mechanical system, but its logarithmic derivative with respect to energy can, as has been pointed out by Rugh [3,4]. Using Gauss's theorem the last integral can be written as

$$W(E)=\int_{\mathcal{H}<E}\vec{\nabla}\cdot\frac{\vec{\nabla}\mathcal{H}}{|\vec{\nabla}\mathcal{H}|^2}\prod_{i=1}^{N} dq_i\,dp_i\,, \tag{2}$$

that is, as an integral over all phase space where the energy is lower than $E$. The derivative with respect to $E$ is again a constant energy integral like Eq. (1) for $W$:

$$\frac{\partial W}{\partial E}=\int \delta(E-\mathcal{H})\vec{\nabla}\cdot\frac{\vec{\nabla}\mathcal{H}}{|\vec{\nabla}\mathcal{H}|^2}\prod_{i=1}^{N} dq_i\,dp_i\,. \tag{3}$$

The ratio is the inverse temperature according to $1/T=\partial S/\partial E$,

$$\frac{\partial W}{\partial E}\bigg/ W(E)=\frac{1}{T}, \tag{4}$$

and defines a microcanonical average, so that the temperature is given by

$$\frac{1}{\mathcal{T}}=\sum_{j}^{2N}\partial_j\frac{\partial_j\mathcal{H}}{|\Sigma_l\partial_l\mathcal{H}|^2}\quad\text{and}\quad\frac{1}{T}=\left\langle\frac{1}{\mathcal{T}}\right\rangle. \tag{5}$$

In this formula the $\partial_j$ are the derivatives with respect to the $2N$ canonical variables $(q_i,p_i)$. Actually, the microcanonical temperature is determined. The difference from the canonical temperature is most noticeable for small systems as has been discussed in greater detail recently by Bannur [5], using very small systems with chaotic dynamics as examples. With the argument given there one also arrives at Eq. (5).

In this paper we show that a formula very similar in structure exists to define the microcanonical temperature as an average for classical Heisenberg spins:

$$\frac{1}{\mathcal{T}}=\sum_j[\vec{S}_j\times\vec{\nabla}_j]\cdot\frac{[\vec{S}_j\times\vec{\nabla}_j]\mathcal{H}}{|\Sigma_l\vec{S}_l\times\vec{\nabla}_l\mathcal{H}|^2}. \tag{6}$$

The sum is over all spins $\vec{S}_j$ and $\vec{\nabla}_j$ is the derivative with respect to its components. Both are three-component vectors and $[\vec{S}_j\times\vec{\nabla}_j]$ is actually an angular momentum operator.

We will test this microcanonical spin temperature for few spins, in a magnetic field and also for many spins, where it reproduces the usual canonical relation between energy and temperature. Further, we want to show its usefulness by testing it together with a molecular dynamics calculation for longer spin chains. In the case that the system size is large, formula (5) simplifies to

$$\mathcal{T}=-\frac{\Sigma_j^N\dot{\vec{S}}_j^2}{4\mathcal{H}} \tag{7}$$

with $\mathcal{H}=\Sigma J_{ij}\vec{S}_i\cdot\vec{S}_j$ and the "velocity" of the spin $\dot{\vec{S}}_j=-\vec{S}_j\times\vec{\nabla}_j\mathcal{H}$, in close analogy to the temperature used in molecular dynamics, $\mathcal{T}=(1/3N)\Sigma_j\vec{p}_j^{\,2}/m$, where the summation is over the momenta of $N$ particles moving in three-dimensional space.

## II. MICROCANONICAL TEMPERATURE FOR CLASSICAL SPIN SYSTEMS

Instead of two canonical variables $q$ and $p$ one has the three components of the angular momentum or spin vector $\vec{S}$.

---

*Electronic address: nurdin@physik.fu-berlin.de

†Electronic address: schotte@hmi.de

However, if these are restricted to always have the same length, in fact there are only two independent variables. With Nambu's notation [6] for the equation of motion as a Jacobian one can deal with these peculiarities in a natural way,

$$\frac{\partial S^i}{\partial t} = -\frac{\partial(S^i,\mathcal{S},\mathcal{H})}{\partial(S^1,S^2,S^3)}, \tag{8}$$

where $\mathcal{S}=\frac{1}{2}[(S^1)^2+(S^2)^2+(S^3)^2]$ guarantees that the size of the angular momentum is conserved. $\mathcal{S}$ put into the last equation instead of $S^i$ gives zero for the time derivative of $\mathcal{S}$, that is, the length of $\vec{S}$ is fixed. In a sense one has now two ''Hamiltonians,'' the squared angular momentum $\mathcal{S}$ and the energy $\mathcal{H}$. The simplest example for a spin Hamiltonian is $\mathcal{H}=-\vec{H}\cdot\vec{S}$ with $H$ the magnetic field. Since the energy is also a conserved quantity, the spin must be on a surface of constant energy in three-dimensional spin space, a plane for the case of a spin in a magnetic field, and at the same time it must be on the sphere with radius $S=|\vec{S}|$. Therefore the orbit is a circle in the case of a magnetic field. The Nambu form Eq. (8) is, of course, nothing else but the standard equation,

$$\partial\vec{S}/\partial t = -\vec{S}\times\vec{\nabla}\mathcal{H} \quad \text{with} \quad \nabla\mathcal{H}=\left(\frac{\partial\mathcal{H}}{\partial S^1},\frac{\partial\mathcal{H}}{\partial S^2},\frac{\partial\mathcal{H}}{\partial S^3}\right), \tag{9}$$

where the vector product guarantees spin and energy conservation, since $\vec{S}\cdot\dot{\vec{S}}=\vec{\nabla}\mathcal{H}\cdot\dot{\vec{S}}=0$. For the case of a spin in a magnetic field this equation reduces to $\partial\vec{S}/\partial t=\vec{S}\times\vec{H}$.

The phase space is the surface of a sphere and for $N$ spins $N$ spheres. In order to use statistical mechanics instead of ''dynamical'' mechanics one has to check that phase space is conserved. With

$$\vec{\nabla}\cdot\partial\vec{S}/\partial t = -\vec{\nabla}\times\vec{S}\cdot\vec{\nabla}\mathcal{H} = -\vec{S}\cdot\vec{\nabla}\times\vec{\nabla}\mathcal{H}=0, \tag{10}$$

the divergence of the flow in phase space generated by the dynamics of Eq. (9) is zero, since $\vec{\nabla}\times\vec{\nabla}\mathcal{H}=0$. In the case of many spins this divergence disappears for each spin separately, as it does for each individual pair of canonical variables $(q_n,p_n)$ in common mechanical systems, that is, $\partial\dot{q}_n/\partial q_n+\partial\dot{p}_n/\partial p_n=0$. Thus a microcanonical temperature definition for a spin system with $N$ spins $S_i$ analogous to a conventional mechanical system [see Eq. (1)] starts with

$$\begin{aligned} W &= \int \delta(E-\mathcal{H})\prod_{i=1}^{N}\delta(S-S_i)\,dS_i^1 dS_i^2 dS_i^3 \\ &= \int \delta(E-\mathcal{H})\prod_{i=1}^{N} do_i = S\int_{\mathcal{H}=E}\frac{dO_{2N-1}}{|\Sigma_l \vec{S}_l\times\vec{\nabla}_l\mathcal{H}|}. \end{aligned} \tag{11}$$

One has only to integrate over the surfaces of the spheres with $S_i=S$ indicated by $\int\Pi_i do_i$, that is a $2N$-dimensional integral. As in Eq. (1) the integral is restricted by $\mathcal{H}=E$ to $2N-1$ dimensions denoted by the ''surface'' element $dO_{2N-1}$. For one spin the last term in Eq. (11) reduces to a line integral $S\int_{\mathcal{H}=E} ds_1/|\vec{S}_1\times\vec{\nabla}_1\mathcal{H}|$. The gradient of the energy $\vec{\nabla}_1\mathcal{H}$ projected on the surface of the sphere $|\vec{S}_1\times\vec{\nabla}_1\mathcal{H}|/S$ has to appear in the denominator, since only the part tangential to the surface of the sphere should be taken into account.

To proceed with two and more spins one has to write the last integral in Eq. (11) in an expanded form as

$$\begin{aligned} W &= S\int_{\mathcal{H}=E}\frac{\Sigma_j[\vec{S}_j\times\vec{\nabla}_j\mathcal{H}]\cdot d\vec{s}_j\Pi_{i\neq j}do_i}{\Sigma_l|\vec{S}_l\times\vec{\nabla}_l\mathcal{H}|^2} \\ &= S\int_{\mathcal{H}<E}\sum_j \vec{\nabla}_j\times\frac{[\vec{S}_j\times\vec{\nabla}_j]\mathcal{H}}{\Sigma_l|\vec{S}_l\times\vec{\nabla}_l\mathcal{H}|^2}\cdot d\vec{o}_j\prod_{i\neq j} do_i, \end{aligned} \tag{12}$$

where use has been made of $[\vec{S}_j\times\vec{\nabla}_j\mathcal{H}]$ being parallel to the line of constant energy, so that the numerator makes the integrand appear as a sum of line integrals amenable to Stokes integral formula. Since the vector character of the surface element $d\vec{o}_j$ can be transferred to the spin $Sd\vec{o}_j=\vec{S}_j do_j$, the last integral can be written in a more transparent way as

$$W(E)=\int_{\mathcal{H}<E}\sum_j [\vec{S}_j\times\vec{\nabla}_j]\frac{[\vec{S}_j\times\vec{\nabla}_j]\mathcal{H}}{\Sigma_l|\vec{S}_l\times\vec{\nabla}_l\mathcal{H}|^2}\prod_i do_i. \tag{13}$$

The integrand is the divergence of a vector field, as can be seen by changing $\vec{S}_j\times\vec{\nabla}_j\ \cdot$ into $\vec{\nabla}_j\cdot\vec{S}_j\ \times$. It has also the general form of the vector field $\vec{X}$ used by Rugh [4] to define microcanonical averages with the property that the scalar product of $\vec{\nabla}\mathcal{H}$ and $\vec{X}$ should be equal to 1.

The volume of phase space with energy $E$ is expressed in Eq. (13) as an integral over all phase space with energy lower than $E$. The derivative with respect to the energy is then

$$\frac{\partial W}{\partial E}=\int \delta(E-\mathcal{H})\sum_j [\vec{S}_j\times\vec{\nabla}_j]\frac{[\vec{S}_j\times\vec{\nabla}_j]\mathcal{H}}{\Sigma_l|\vec{S}_l\times\vec{\nabla}_l\mathcal{H}|^2}\prod_i do_i, \tag{14}$$

again a constant energy integral like $W$ in Eq. (11). Since the inverse temperature is $1/T=(\partial W/\partial E)/W$, the function $1/\mathcal{T}$ to be averaged is the integrand of Eq. (14) given already in Eq. (6).

With $\vec{\mathcal{L}}_j=[\vec{S}_j\times\vec{\nabla}_j]$ and the summation from 1 to $N$ the integrand of Eq. (14) can be split into two terms,

$$\frac{1}{\mathcal{T}}=\frac{\Sigma_j\vec{\mathcal{L}}_j^2\mathcal{H}}{\Sigma_l(\vec{\mathcal{L}}_l\mathcal{H})^2}+\sum_j (\vec{\mathcal{L}}_j\mathcal{H})\vec{\mathcal{L}}_j\frac{1}{\Sigma_l(\vec{\mathcal{L}}_l\mathcal{H})^2}, \tag{15}$$

where the last term for large $N$ is of the order $1/N$, since $\mathcal{H}$ connects the spin $\vec{S}_i$ only to neighboring spins and the differential operator $\mathcal{L}_j$ produces nonzero contributions only for $l=j$ and for $l$ close to $j$. A single sum in the numerator and a double sum in the denominator gives then only a contribution that scales as $\propto 1/N$. The meaning of Eq. (6) or Eq. (15) can best be clarified by simple examples discussed in the next section.

## III. PARAMAGNET AS AN EXAMPLE

With paramagnets it is easiest to test the spin temperature formulas (6) and (15) derived in the preceding section. In paramagnets as in ideal gases there is no interaction and the Hamiltonian is simply $\mathcal{H}_{pM} = -H\Sigma_i^N S_i^3$, where $H$ is the magnetic field parallel to $\vec{S}^3$. One obtains

$$\sum_j [\vec{S}_j \times \vec{\nabla}_j]\mathcal{H}_{pM} = -H\{(S_1^2, -S_1^1, 0), \ldots, (S_N^2, -S_N^1, 0)\}, \tag{16}$$

which is a $3N$-dimensional vector, and further

$$\sum_j [\vec{S}_j \times \vec{\nabla}_j]^2 \mathcal{H}_{pM} = 2H \sum_j S_j^3 = -2\mathcal{H}_{pM}. \tag{17}$$

This could be inferred without explicit calculations, since $-[\vec{S}_j \times \vec{\nabla}_j]^2$ is the square of angular momentum operator (used in quantum mechanics) and should give $l(l+1)$ with $l=1$ if applied to $S_j^3$, since $S_j^3$ is a component of a vector with eigenvalue 1. For the denominator of Eq. (6) one has to square Eq. (16): $|\Sigma_j[\vec{S}_j \times \vec{\nabla}_j]\mathcal{H}_{pM}|^2 = H^2\Sigma_j[S_j^2 - (S_j^3)^2]$. One obtains for the inverse temperature $1/\mathcal{T}$ the first term of the following equation:

$$\frac{1}{\mathcal{T}_{pM}} = \frac{-2\mathcal{H}_{pm}}{H^2\Sigma_l[S^2-(S_l^3)^2]} - \frac{2\ \ \Sigma_j S_j^3[S^2-(S_j^3)^2]}{H|\Sigma_l[S^2-(S_l^3)^2]|^2}. \tag{18}$$

The second term is obtained by applying in Eq. (15) $\vec{\mathcal{L}}_j = [\vec{S}_j \times \vec{\nabla}_j]$ to the denominator, that is, $\vec{\mathcal{L}}_j \Sigma_l[S^2-(S_l^3)^2] = -2S_j^3(S_j^2, -S_j^1, 0)$. Making use of Eq. (16) one gets finally the numerator of the second term of Eq. (17). For a large number of spins $N$, this second term becomes small since the numerator is proportional to $N$ while the denominator is proportional to $N^2$. Therefore it can be interpreted as a finite size correction.

For small magnetic fields the first term of Eq. (18) alone gives Curie's susceptibility formula. The energy is $\mathcal{H}_{pM} = -H\mathcal{M}$ with the magnetization $\mathcal{M} = \Sigma_i S_i^3$. If the number of spins $N$ is large then it is of advantage to take the average of the inverse $T = \langle \mathcal{T}_{pM} \rangle$ instead of $\langle 1/\mathcal{T}_{pM} \rangle$, that is, for the temperature directly with

$$\mathcal{T}_{pM} \approx -\frac{H^2\Sigma_{i=1}^N[S^2-(S_i^3)^2]}{2\mathcal{H}_{pM}}, \tag{19}$$

where the second and smaller term in Eq. (17) has been neglected. Using this form and for the average $\langle (S_i^3)^2 \rangle = \frac{1}{3}S^2$ which is valid for small $H$, one obtains

$$\mathcal{M} = N\frac{S^2}{3T}H, \tag{20}$$

with the correct value $NS^2/3$ for Curie's constant.

Using the canonical ensemble one can check Eq. (19) also for larger $H$. With $S_3 = S\cos\theta$ and $h = HS/T$ the canonical averages $I_n = \langle (\cos\theta)^n \rangle$ for $n = 0,1,2$ are $I_0 = \sinh h/h$, $I_1 = \cosh h/h - \sinh h/h^2$, and $I_2 - I_0 = -2I_1/h$. Since the numerator of Eq. (19) is, as before, $\mathcal{H}_{pM} = -H\mathcal{M}$ and the mean value of the denominator $\Sigma_i \langle S^2 - (S_i^3)^2 \rangle = NS^2(I_0 - I_2)/I_0$, one obtains with $\langle \mathcal{T}_{pM} \rangle = T$ for the magnetization $\mathcal{M}$, correctly,

$$\frac{\mathcal{M}}{N} = h\frac{I_1}{I_0} = \coth h - \frac{1}{h}, \tag{20$'$}$$

as a function of $h = HS/T$.

For small $N$ Eq. (18) should give the microcanonical temperature. For only one spin the total phase space is $4\pi S^2$, which reduces for constant energy $E = -SH\cos\theta$ to $W_1 = 2\pi S/H$. The phase space at constant energy for one spin is independent of energy and therefore according to Eq. (4) the inverse of the microcanonical temperature zero. Indeed $1/\mathcal{T}_1 = 0$ according to Eq. (18) if the sums are reduced to one term.

For two spins the phase space at constant energy (to simplify the notation $S=1$) is

$$\begin{aligned} W_2 &= \int\int dz_1 dz_2 \delta(z_1 + z_2 + E/H) \\ &= (2 - |E/H|) \ \text{ for } \ |E/H| < 2, \end{aligned} \tag{21}$$

where $z_{1/2} = S_{1/2}^3$, the component of $\vec{S}_{1/2}$ in the magnetic field direction. The limits for $z_1$ are $-1 < z_1 < 1$ and since $z_2 = -z_1 - E/H$ the constraint for $z_2$ is $-1 < z_2 < 1 - E/H$ for $E/H > 0$. With Eq. (4) the temperature is then

$$T = -\text{sgn}(E/H)(2 - |E/H|). \tag{22}$$

To compare with Eq. (18) rewritten for two spins with $S_{1/2}^3 = z_{1/2}$ and $S^2 = 1$,

$$\begin{aligned} \frac{1}{\mathcal{T}_2} &= \frac{2}{H}\left(\frac{z_1+z_2}{2-z_1^2-z_2^2} - \frac{z_1(1-z_1^2)+z_2(1-z_2^2)}{2-z_1^2-z_2^2}\right) \\ &= \frac{2}{H}\frac{(z_1+z_2)(1-z_1z_2)}{2-z_1^2-z_2^2}, \end{aligned} \tag{23}$$

again one has to integrate to determine the microcanonical average. To this end one puts $\eta = z_1 + z_2$ and $\zeta = z_1 - z_2$ so that $dz_1dz_2 = d\zeta d\eta/2$. With $\epsilon = E/H$ one gets

$$\begin{aligned} &\int_{-1}^{1}\int_{-1}^{1} dz_1 dz_2 \delta(z_1+z_2+\epsilon)/\mathcal{T}_2 \\ &\quad = -2\epsilon\int_{|\epsilon|-2}^{2-|\epsilon|} d\zeta \frac{4-\epsilon^2+\zeta^2}{(4-\epsilon^2-\zeta^2)^2} = -\text{sgn}(\epsilon), \end{aligned} \tag{24}$$

because with $\eta = z_1 + z_2 = -\epsilon$ the second variable $\zeta = z_1 - z_2$ is limited to the interval $2 - |\epsilon| > \zeta > -2 + |\epsilon|$. For the average $\langle 1/\mathcal{T}_2 \rangle = 1/T$ one has to divide the last result by $W_2$ given by Eq. (21) so that in fact the microcanonical temperature (22) is found.

## IV. SPIN CHAIN

The Hamiltonian for the Heisenberg model is $\mathcal{H}_H = \Sigma'_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j$ where the summation is over spin pairs $\{i,j\}$ connected by the exchange interaction. The corresponding expression for the temperature according to Eq. (15) is

$$\frac{1}{\mathcal{T}_H}=\frac{-4\mathcal{H}}{\Sigma_l(\vec{\mathcal{L}}_l\mathcal{H})^2}+\frac{2\Sigma'_{ij}J_{ij}\{\vec{S}_i\cdot\vec{S}_j(\mathcal{L}_i\mathcal{H}-\mathcal{L}_j\mathcal{H})^2+(\vec{S}_i\cdot\vec{\mathcal{L}}_j\mathcal{H})(\vec{S}_j\cdot\vec{\mathcal{L}}_i\mathcal{H})\}}{\Sigma_l(\vec{\mathcal{L}}_l\mathcal{H})^2} \tag{25}$$

with $\vec{\mathcal{L}}_j=[\vec{S}_i\times\vec{\nabla}_i]$. The derivation is similar to the one for the paramagnet [Eq. (18)] in the last section. The second term is rather complicated; however, for large spin systems it is sufficient to consider only the first term and its inverse

$$\mathcal{T}_H=-\sum_l(\vec{\mathcal{L}}_l\mathcal{H})^2/(4\mathcal{H}), \tag{26}$$

which is close to the kinetic temperature used in molecular dynamics, when written in the form (7). We used this formula to calculate the temperature by integrating the equation of motion for a spin chain of length $N$,

$$\partial\vec{S}_j/\partial t=-\vec{S}_j\times\vec{\nabla}_j\mathcal{H}_{ch}\quad\text{with}\quad\mathcal{H}_{ch}=J\sum_{j=1}^{N-1}\vec{S}_j\cdot\vec{S}_{j+1}, \tag{27}$$

and compared it to the energy relation (see Fisher [7])

$$E=(1-N)[J\coth(J/T)-T] \tag{28}$$

(see Fig. 1). The energy $E$ is fixed and one finds numerically the temperature $T=\langle\mathcal{T}_H\rangle$ using Eq. (26) whereas in the canonical relation $T$ is fixed and the energy is determined as an average. Since in the integration process $\partial\vec{S}_j/\partial t=-\vec{\mathcal{L}}_J\mathcal{H}_H$ is calculated anyway, the additional determination of the temperature is easy.

There is one difficulty hidden in the dynamical approach to temperature, since in addition to the energy additional conserved quantities could appear [8]. For the case of the isotropic Heisenberg model the total spin $\Sigma_i\vec{S}_i$ is a conserved quantity. With a microcanonical Monte Carlo approach such a problem could be circumvented. Here we have taken an initial spin configuration with total spin zero. Pairs of spins oriented in opposite directions which have an angle ±$\alpha$ to the $z$ direction allow the energy variation used in the simulations. For the temperature average plotted in the inset of Fig. 1 all time steps up to the time $t$ are taken.

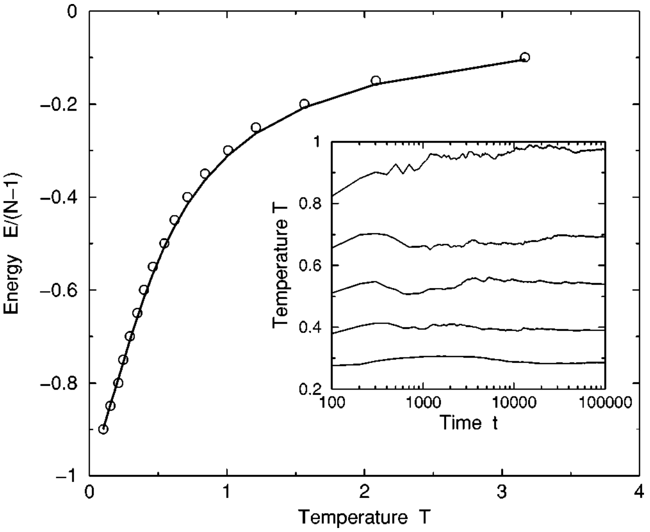

FIG. 1. Relation between temperature and energy for a chain of $N=32$ spins: circles are averages according to Eq. (26), solid line to compare with Eq. (28), and $J=1$. The inset shows the fluctuations of the temperature average as a function of time for different energies.

## V. CONCLUDING REMARKS

We have shown that Rugh's microcanonical temperature definition can be carried over to classical spin systems and we think it could actually be used there in molecular dynamics simulations. The same recipe could also be applied to simulations where the magnetization instead of the energy is constant. With the determination $(\partial S/\partial M)_T$ similar to $(\partial S/\partial E)_M$ discussed, one could make use of the thermodynamic relation $H=(\partial E/\partial M)_T-T(\partial S/\partial M)_T$ and calculate the magnetic field $H$. There are other possibilities for generalizations, like higher derivatives with respect to energy, leading in the next step to the specific heat (see Rugh [4]). In a microcanonical simulation the fluctuations of the $z$ component of the energy $\delta E_{||}$ defined by $\mathcal{H}_H^{||}=\Sigma'_{ij}J_{ij}S_i^3S_j^3$ would determine the specific heat $C$, making use of the connection between canonical and microcanonical fluctuations. A formula of the type found by Lebowitz, Percus, and Verlet [9] is for an isotropic Heisenberg system $\langle(\delta E_{||})^2\rangle_E=\frac{2}{9}T^2C$ [10], where the subscript $E$ indicates the microcanonical average with constant total energy.

## ACKNOWLEDGMENTS

We thank Peter Névir for pointing out Nambu's formulation of mechanics with three canonical variables. W.B.N. thanks DAAD for financial support.

---

[1] A. I. Khinchin, *Mathematical Foundations of Statistical Mechanics* (Dover, New York, 1949).
[2] K. Huang, *Statistical Mechanics* (John Wiley & Sons, New York, 1963).
[3] H. H. Rugh, Phys. Rev. Lett. **78**, 772 (1997).
[4] H. H. Rugh, J. Phys. A **31**, 7761 (1998).
[5] V. M. Bannur, Phys. Rev. E **58**, 407 (1998).
[6] Y. Nambu, Phys. Rev. D **7**, 2405 (1973).
[7] M. E. Fisher, Am. J. Phys. **32**, 343 (1964).
[8] J. R. Ray and H. Zhang, Phys. Rev. E **59**, 4781 (1999).
[9] J. L. Lebowitz, J. K. Percus, and L. Verlet, Phys. Rev. **153**, 250 (1967).
[10] The formula needed is $\langle(\delta E_1)^2\rangle_E=\langle(\delta E_2)^2\rangle_E=T^2C_1C_2/(C_1+C_2)$ with $C_1+C_2$ the total specific heat to be determined.