Ratio of canonical and microcanonical temperatures of a vibratory antiferromagnetic Ising chain

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The ratio of canonical and microcanonical temperatures T_c/T_μ of a vibratory antiferromagnetic Ising chain with N spins is given by analytical calculation. The result is $T_c/T_\mu = 1 + O(N^{-1})$, which is consistent with the natural assumption given by Rugh.

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A quite simple statistical principle claims that the measured value of a thermodynamic observable of a system and the ensemble average or the time average of the observable are identical at the thermodynamic limit. Some examples of the principle were given in canonical ensemble, which describes the thermodynamics of a closed system [1]. For an isolated classical Hamiltonian system, the time average of an observable of a system may be replaced by the average of the microcanonical ensemble. In present understanding, there is an equivalent canonical ensemble for the system, which gives the same average values for all observables at the thermodynamic limit [1]. A typical observable is temperature T. In a canonical ensemble, the temperature is a free parameter, which determines the internal energy $U = U(T_c)$ of a system. But in a microcanonical ensemble the energy E of a system is a free parameter, and the temperature is an observable to be calculated as $T_\mu = T_\mu(E)$ [1,2]. Here the subscripts c and μ represent the canonical and the microcanonical ensemble averages, respectively. The equivalence of the two ensembles means that $T_\mu = T_c$ for $E = U$ at the thermodynamic limit. Rugh proposed a method calculating the reciprocal temperature in a microcanonical ensemble and deduced an equation of the ratio T_c/T_μ for some classical interaction model [3,4]. He gave the result that the ratio T_c/T_μ differs from one by a term of order N^{-1} under the natural assumption on the fluctuations in the kinetic energy [4,5]. However, the assumption, up to now, lacks a rigorous argument for a system with interaction because of the difficulty in the analytical calculation.

One-dimension ferromagnetic and antiferromagnetic chains have been widely considered in statistical physics and nonlinear physics [1,2,6,7]. In this paper, we give a descriptive example to calculate the ratio T_c/T_μ of a classical Hamiltonian system, which is an antiferromagnetic Ising chain with N spins and its sites vibrate harmonically. Our model is closer to a practical system. The ratio T_c/T_μ is given by a rigorous analytical calculation. The result is $T_c/T_\mu = 1 + O(N^{-1})$, which is consistent with the natural assumption [4,5].

The Ising chain has N sites labeled by q_i, $i = 1, \ldots, N$ and there is a spin S_i on every site. Moreover, every site vibrates as a three-dimension harmonic oscillator. Then the total Hamiltonian of the system is

$$H = H_r + H_b. \tag{1}$$

$H_b\{S_i\}$ is the Hamiltonian of the one-dimensional antiferromagnetic Ising chain such that

$$H_b = J\sum_{i=1}^{N}(S_iS_{i+1}+1)/4. \tag{2}$$

Here, we take $S_{N+1} = S_1$. The Hamiltonian $H_r(q,p)$ of the harmonic vibration of the sites is

$$H_r(q,p) = \sum_{i=1}^{N}(\vec{p}_i^{\,2}/2 + \vec{q}_i^{\,2}/2). \tag{3}$$

For a closed isolated antiferromagnetic Ising chain as described by Eq. (2), let the number of $S_iS_{i+1} = -1$ be M, and the number of $S_iS_{i+1} = 1$ be $N - M$. We have the energy of the chain such that

$$E_b(M,N) = J(N-M)/2. \tag{4}$$

The corresponding configuration number is

$$\Gamma(M,N) = 2C_N^M. \tag{5}$$

Setting $M/N = a$ and according to the definition $\beta_\mu = \partial \ln\Gamma/\partial E_b$, we have the reciprocal temperature of the chain in a microcanonical ensemble as follows:

$$\beta_\mu = \lim_{N\to\infty}\frac{\ln\Gamma(M+1,N) - \ln\Gamma(M,N)}{E_b(M+1,N) - E_b(M,N)} = -\frac{2}{J}\ln\frac{1-a}{a}. \tag{6}$$

The above result means that the chain has a negative temperature if $M < N/2$, but a positive temperature if $M > N/2$.

The vibratory one-dimensional antiferromagnetic chain with Hamiltonian (1) has the total configuration number corresponding to the energy $E = N\varepsilon$,

$$\Omega(E) = \sum_{M=0}^{N}\Omega(M) = \sum_{M=0}^{N} A\left[E - \frac{J(N-M)}{2}\right]^{3N} C_N^M, \tag{7}$$

where A is a constant, and $E \geqslant J(N-M)/2$ since the Hamiltonian $H_r \geqslant 0$ in Eq. (3). Here, we use the bulk volume rather than surface area to define the function $\Omega(M)$ because they are the same for large N. The Boltzmann constant and Planck constant are both taken to be unity in our calculation.

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For the chain as described by Eq. (1), the total entropy is the sum of the vibratory part and the antiferromagnetic part of the Ising chain in the thermodynamic limit. The reciprocal temperature can be given by the thermal equilibrium of the two parts such that

$$-\frac{2}{J}\ln\frac{1-\bar{a}}{\bar{a}}=\beta_\mu=\frac{3}{\varepsilon-\frac{J}{2}(1-\bar{a})}, \tag{8}$$

where $\bar{a}=\bar{M}/N$, and $\bar{M}$ determines the largest term $\Omega(\bar{M})$ in the sum (7). It is noted that $\bar{a}$ is independent of the total site number N. The condition of positive temperature means $\bar{M}>N/2$ and $\bar{M}<N$ for the finite temperature. Consequently, we can obtain

$$\bar{M}=\frac{Ne^{3J/[2\varepsilon-J(1-\bar{a})]}}{1+e^{3J/[2\varepsilon-J(1-\bar{a})]}}=\frac{Ne^{J\beta_\mu/2}}{1+e^{J\beta_\mu/2}} \tag{9}$$

and

$$\bar{E}_b=\frac{JN}{1+e^{3J/[2\varepsilon-J(1-\bar{a})]}}=\frac{JN}{1+e^{J\beta_\mu/2}}. \tag{10}$$

Using the Stirling formula, we can write the configuration number $\Omega(M)$ in the form as

$$\Omega(M)=AC_N^M\left[E-\frac{J(N-M)}{2}\right]^{3N}=Be^{Nh(M)}, \tag{11}$$

where B is independent of M, i.e.,

$$B=\frac{AN^{N+1/2}}{\sqrt{2\pi}(N-\bar{M})^{N-\bar{M}+1/2}\bar{M}^{\bar{M}+1/2}}E^{3N}\left[1-\frac{J}{2}(1-\bar{a})\right]^{3N}, \tag{12}$$

and

$$\begin{aligned}h(M)=&3\ln\left(1+\frac{J\beta_\mu}{2}\frac{M-\bar{M}}{3N}\right)+\frac{J\beta_\mu}{2N}(\bar{M}-M)\\&-\left(1-\frac{M-1/2}{N}\right)\ln\left[1+\frac{\bar{M}-M}{N(1-\bar{a})}\right]\\&-\frac{M+1/2}{N}\ln\left(1+\frac{M-\bar{M}}{\bar{M}}\right).\end{aligned} \tag{13}$$

Taking $a-\bar{a}=t$, the total configuration number $\Omega(E)$ can be written in the integral form by Euler's formula,

$$\begin{aligned}\Omega(E)=&\sum_{M=0}^{N}\Omega(M)\\=&O\left\{NB\int_{-\bar{a}}^{1-\bar{a}}\left(1-\frac{t}{1-\bar{a}}\right)^{-1/2}\left(1+\frac{t}{\bar{a}}\right)^{-1/2}e^{Nh(t)}dt\right\},\end{aligned} \tag{14}$$

where

$$\begin{aligned}h(t)=&3\ln\left(1+\frac{J\beta_\mu}{6}t\right)-\frac{J\beta_\mu}{2}t-(1-\bar{a}-t)\ln\left(1-\frac{t}{1-\bar{a}}\right)\\&-(\bar{a}+t)\ln\left(1+\frac{t}{\bar{a}}\right).\end{aligned} \tag{15}$$

The reciprocal temperature of the system denoted in a microcanonical ensemble is given by the definition $1/T_\mu(E)=\partial\ln\Omega(E)/\partial E$. According to the definition, we can directly obtain the following result

$$\frac{1}{T_\mu(E)}=3N\left\langle\frac{1}{H_r(q,p)};E\right\rangle_\mu. \tag{16}$$

This equation is the same as that given by Rugh [3,4]. The symbols $\langle C\rangle_\mu$ and $\langle C\rangle_c$ represent the microcanonical ensemble and canonical ensemble averages of an observable C, respectively.

The temperature of the system in the canonical ensemble is

$$T_c(E)=\frac{1}{3N}\langle H_r(q,p);E\rangle_c. \tag{17}$$

The ratio of the temperatures can be expressed as follows:

$$\frac{T_c(E)}{T_\mu(E)}=\langle H_r(q,p);E\rangle_c\left\langle\frac{1}{H_r(q,p)};E\right\rangle_\mu. \tag{18}$$

So, we have

$$\begin{aligned}T_c(E)/T_\mu(E)=&\langle H-H_b;E\rangle_c\left\langle\frac{1}{E-H_b};E\right\rangle_\mu\\=&(U-\langle H_b\rangle_c)\mu_1\left(\frac{1}{E-H_b}\right),\end{aligned} \tag{19}$$

where $\mu_1(x)$ represents the first-order moment of x. Furthermore, the ratio of the temperatures can be written as

$$\begin{aligned}T_c(E)/T_\mu(E)=&\langle H-H_b;E\rangle_c\left\langle\frac{1}{E-H_b};E\right\rangle_\mu\\=&\frac{U-\langle H_b\rangle_c}{E-\bar{E}_b}\mu_1\left(\frac{1-\bar{E}_b/E}{1-H_b/E}\right)\\=&\frac{U-\langle H_b\rangle_c}{E-\bar{E}_b}\mu_1[1+g(t)]\\=&\frac{U-\langle H_b\rangle_c}{E-\bar{E}_b}+O\{\mu_1[g(t)]\},\end{aligned} \tag{20}$$

where the function $g(t)$ is defined as

$$\frac{1-\bar{E}_b/E}{1-H_b/E}=\frac{1}{1+\frac{J\beta_\mu}{6}\frac{M-\bar{M}}{N}}=1-\frac{\frac{J\beta_\mu}{6}t}{1+\frac{J\beta_\mu}{6}t}=1+g(t). \tag{21}$$

According to Euler's formula as used in Eq. (14), we have

$$
O\{\mu_1[g(t)]\} = O\left[\frac{NB\int_{-\bar{a}}^{1-\bar{a}}\left(1-\frac{t}{1-\bar{a}}\right)^{-1/2}\left(1+\frac{t}{\bar{a}}\right)^{-1/2} g(t)e^{Nh(t)}dt}{\Omega(E)}\right]. \tag{22}
$$

To calculate $O\{\mu_1[g(t)]\}$ in Eq. (22), we can use the Laplace formula: if $f(t)$ and $h(t)$ are analytical at $t\in[0,b]$, and $h(t)$ has the largest value $h(0)$ at $t=0$, and $h'(0)=h''(0)=\cdots=h^{(p-1)}(0)=0$, $h^{(p)}(0)\neq 0$; $f(0)=f'(0)=\cdots=f^{(q-1)}(0)=0$, $f^{(q)}(0)\neq 0$, then

$$
\int_0^b f(t)e^{Nh(t)}dt = e^{Nh(0)}\left[\frac{a_1}{N^{(q+1)/p}}+\frac{a_2}{N^{(q+2)/p}}+\frac{a_3}{N^{(q+3)/p}}+\cdots\right], \tag{23}
$$

where a_1, a_2, a_3 are determined by $a_i=\int_0^\infty A_i(\omega)e^{-\omega}d\omega$, $i=1, 2, 3, \ldots$, with

$$
A_1(\omega)=\frac{1}{p}\left[-\frac{p!}{h^{(p)}(0)}\right]^{(q+1)/p}\frac{f^{(q)}(0)}{q!}\omega^{(q+1)/p-1},
$$

$$
A_2(\omega)=\frac{1}{p}\left[-\frac{p!}{h^{(p)}(0)}\right]^{(q+2)/p}\left[\frac{f^{(q+1)}(0)}{(q+1)!}-\frac{f^{(q)}(0)h^{(p+1)}(0)}{q!(p+1)h^{(p)}(0)}\omega\right]\omega^{(q+2)/p-1},
$$

$$
\vdots\,. \tag{24}
$$

In our calculation, the function $h(t)$ in Eq. (15) has $h(0)=h'(0)=0$, $h''(0)=-[(J\beta_\mu)^2/12+1/\bar{a}(1-\bar{a})]$, and $h'''(0)=(J\beta_\mu)^3/36-1/(1-\bar{a})^2+1/\bar{a}^2$ at $t=0$, which means $p=2$. The function $f(t)=[1-t/(1-\bar{a})]^{-1/2}(1+t/\bar{a})^{-1/2}g(t)$ has $f(0)=0$, $f'(0)=-J\beta_\mu/6$, and $f''(0)=(J\beta_\mu)^2/18-J\beta_\mu(2\bar{a}-1)/6\bar{a}(1-\bar{a})$, which means $q=1$. So we have

$$
NB\int_{-\bar{a}}^{1-\bar{a}}f(t)e^{Nh(t)}dt = NB\left[\int_0^{1-\bar{a}}f(t)e^{Nh(t)}dt+\int_0^{\bar{a}}f(-t)e^{Nh(-t)}dt\right] = C_1BN^{-1/2}+O(N^{-1}), \tag{25}
$$

with

$$
C_1=\left[\frac{2}{(J\beta_\mu)^2/12+1/\bar{a}(1-\bar{a})}\right]^{3/2}\times\left\{\left[\frac{(J\beta_\mu)^2}{36}-\frac{J\beta_\mu(2\bar{a}-1)}{12\bar{a}(1-\bar{a})}\right]\frac{\sqrt{\pi}}{2}-\frac{\frac{J\beta_\mu}{6}\left[\frac{(J\beta_\mu)^3}{36}-\frac{1}{(1-\bar{a})^2}+\frac{1}{\bar{a}^2}\right]\sqrt{\pi}}{4\left[\frac{(J\beta_\mu)^2}{12}+\frac{1}{\bar{a}(1-\bar{a})}\right]}\right\}.
$$

Similarly, we can obtain

$$
\Omega(E)=NB\int_{-\bar{a}}^{1-\bar{a}}\left(1-\frac{t}{1-\bar{a}}\right)^{-1/2}\left(1+\frac{t}{\bar{a}}\right)^{-1/2}e^{Nh(t)}dt = C_2B\sqrt{N}+O(1), \tag{26}
$$

with

$$
C_2=\sqrt{\frac{2\pi}{(J\beta_\mu)^2/12+1/\bar{a}(1-\bar{a})}}.
$$

At last, we get

$$
\mu_1[g(t)]=\frac{NB\left[\int_0^{1-\bar{a}}f(t)e^{Nh(t)}dt+\int_0^{\bar{a}}f(-t)e^{Nh(-t)}dt\right]}{\Omega(E)} = \frac{C_1}{C_2}N^{-1}+O(N^{-3/2}). \tag{27}
$$

If setting $U=E$, then $\langle H_b\rangle_c=\bar{E}_b$. Equation (20) leads to the result $T_c/T_\mu=1+(C_1/C_2)N^{-1}+O(N^{-3/2})$, which is consistent with the natural assumption [4,5]. The above discussion shows that the temperature of a microcanonical ensemble and that of a canonical ensemble are equivalent for a vibratory antiferromagnetic Ising chain at the thermodynamic limit.

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