# ENTROPY AND TEMPERATURE OF THE THREE-LEVEL SYSTEM: THE MICRO-CANONICAL ENSEMBLE METHOD

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Based on the micro-canonical ensemble (MCE) theory and the method of steepest descend, we rederive a formula for the entropy and the temperature in the general three-level system. Compared with the results commonly based on the canonical ensemble (CE) method, we verify the correctness of our method. The solving process could be expanded in the multi-level systems. The results could be the perturbation-theory foundation for further discussion on some complex interacting multi-level systems.

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## 1. Introduction

The ensemble theory in the $2J+1$-level system plays an important role in investigating the atom with spin $J$ in magnetic field [1]. For example, using the canonical ensemble (CE), the researchers have discussed the ferromagnetic property and the negative-temperature system [2–6]. In atomic physics, the negative-temperature ensemble is possible in an optical lattice and enables the attainment of the Bose–Einstein condensation (BEC) phase transition by evaporation of the lowest-energy particles [7]. In the researches on BEC, the calculation on three-level system is basal and crucial [8, 9]. If all thermodynamic functions could be apparently expressed by the energy $E$ or the occupation numbers of different level $x_i$, it will be more convenient to make both theoretical prediction and experimental comparison. The micro-canonical ensemble (MCE) system method, where the particle number and energy are conserved, would be a perfect tool. However, excluding the simple 2-level system [1], few researchers use the MCE method to solve the $n$-level system when $n \geq 3$. In this paper, we try to aim at this problem where $n = 3$.

In Sec. 2, based on the micro-canonical ensemble theory and the method of steepest descend, we derive a new formula for the entropy and the temperature in a general three-level system. In Sec. 3, compared with the results commonly based on the canonical ensemble method, we verify the correctness of our method.

## 2. Entropy and temperature of the three-level system based on the micro-canonical ensemble method

The Hamiltonian in a three-level system reads

$$H = \sum_{i=1}^{N} \sigma_i \epsilon, \sigma_i = -1, 0, 1 \,. \tag{1}$$

For a magnetic system, $\epsilon = \mu_B B \equiv g_l \mu_0 B$, where $g_l$ is the Landé coefficient, $\mu_0$ is the Bohr magneton and $B$ is the magnetic flux density. In the micro-canonical ensemble system, the total number $N$ of particles and the total energy $E$ are conserved. We have the tacit assumption that the number of particles is very large in the thermodynamic limit. It is known that

$$x_1 + x_0 + x_{-1} = N\,; \qquad (x_1 - x_{-1})\epsilon = E\,. \tag{2}$$

For simplification, one can rewrite $N \approx 2[\frac{N}{2}] \equiv 2k_0, N_1 \approx [\frac{E}{\epsilon}] \approx 2[\frac{N_1}{2}] \equiv 2k_1$. Here, $[\zeta]$ denotes the integer-valued function of $\zeta$. After solving the above equation, one can get $x_1 = k_0 + k_1 - x, x_{-1} = k_0 - k_1 - x, x_0 = 2x, 0 \leq x \leq (k_0 - k_1)$.

The number of microstates $\Omega(N, E)$ reads

$$\Omega(N, E) = (N!) \sum_{x=0}^{k_0 - k_1} \frac{1}{(k_0 + k_1 - x)!(k_0 - k_1 - x)!(2x)!}\,. \tag{3}$$

Introducing $A \equiv k_0 - k_1, B \equiv k_0 + k_1$, and using Stirling's formula meaning $m! \approx \exp(m \ln m - m)$, we have

$$\Omega(N, E) \approx N!\, \mathrm{e}^N \int_0^A \exp\{-[(A-x)\ln(A-x) + (B-x)\ln(B-x) + 2x\ln(2x)]\}\mathrm{d}x\,. \tag{4}$$

On the other hand, considering the method of steepest decent [1], which reads

$$\int_{-\infty}^{+\infty} \mathrm{e}^{\Phi(x)}\mathrm{d}x \approx \sqrt{\frac{2\pi}{|\Phi''(x_{\max})|}}\mathrm{e}^{\Phi(x_{\max})}\,, \qquad \Phi(x) \equiv N\phi(x)\,, \tag{5}$$

one can analytically solve the number of microscopic states $\Omega(N,E)$. Here, $x_{\max}$ is the maximum point of $\Phi(x)$. It is to say that $\Phi'(x_{\max})=0, \Phi''(x_{\max})<0$. The method of steepest descent means the saddle point integration [1]. In statistical physics, we frequently encounter sums or integrals of exponential variables. Preforming such sums or integrals in the thermodynamic limit is considerably simplified due to the summation of exponential quantities. Considering the sum

$$\delta = \sum_{i=1}^{\omega} \psi_i, 0 \leq \psi_i \sim O(\exp(N\phi_i))\,, \qquad \omega \propto N^r\,, \tag{6}$$

one can write

$$\psi_{\max} \leq \delta \leq \omega\psi_{\max} \Rightarrow \lim_{N\to\infty} \frac{\ln\delta}{N} = \frac{\ln\psi_{\max}}{N} = \phi_{\max}\,. \tag{7}$$

Considering the narrow fluctuations of energy in micro-canonical ensemble, $\Phi(x) = \Phi(x_{\max}) + \frac{1}{2}\Phi''(x_{\max})(x-x_{\max})^2 + O((x-x_{\max})^3)$, here $\Phi''(x_{\max}) \simeq N$. The narrow energy window provides the leading value for the Gaussian integral.

Therefore, we have

$$\Phi'(x) = \ln(A-x) + \ln(B-x) - 2\ln(2x)\,; \quad \Phi''(x) = -\left[\frac{1}{(A-x)} + \frac{1}{(B-x)} + \frac{2}{x}\right]. \tag{8}$$

and the root $x_{\max}$ reads

$$x_{\max} = \frac{\sqrt{A^2+B^2+14AB}-(A+B)}{6} = \frac{\sqrt{N^2-0.75\left(\frac{E}{\epsilon}\right)^2}-0.5N}{3}\,. \tag{9}$$

Thus, we get

$$\begin{aligned} \Phi(x_{\max}) &= -[2A\ln(2x_{\max}) + (B-A)\ln(B-x_{\max})] \\ &= -\left\{(B+A)\ln(2x_{\max}) + \left[(B-A)\ln\left(\frac{B-x_{\max}}{2x_{\max}}\right)\right]\right\} \\ &= -\left\{N\ln(2x_{\max}) + \left[\frac{E}{\epsilon}\ln\left(\frac{B-x_{\max}}{2x_{\max}}\right)\right]\right\}. \end{aligned} \tag{10}$$

For simplification, after introducing the reduce energy $\tilde{E} \equiv s = \frac{E}{N\epsilon}$, one can obtain

$$\begin{aligned} \Phi(x_{\max}) = & -N\left\{\ln N - \ln 3 + \ln\left(\sqrt{4-3s^2}-1\right)\right. \\ & \left. + s\ln\left(\frac{4+3s-\sqrt{4-3s^2}}{\sqrt{4-3s^2}-1}\right) - s\ln 2\right\}. \end{aligned} \tag{11}$$

Since $\ln \Phi''(x_{\max}) \simeq \ln N \ll N$, we know the entropy which reads $S = k_{\rm B} \ln \Omega(N,E) \simeq k_{\rm B}[N \ln N + \Phi(x_{\max})]$. Here, $k_{\rm B}$ is the Boltzmann constant. Let $k_{\rm B} \equiv 1$. The entropy reads

$$\begin{aligned} S &= N\left[\ln 3 + s\ln 2 + (s-1)\ln\left(\sqrt{4-3s^2}-1\right) - s\ln\left(4+3s-\sqrt{4-3s^2}\right)\right] \\ &\equiv N\eta(s)\,. \end{aligned} \tag{12}$$

The temperature is defined by the following formula:

$$\frac{1}{T} \equiv \left.\frac{\partial S}{\partial E}\right|_N = \left.\frac{1}{\epsilon}\frac{\partial \eta(s)}{\partial s}\right|_N = \frac{1}{\epsilon}\frac{\partial \eta}{\partial s} \quad \text{or} \quad T = \epsilon\left(\frac{\partial \eta}{\partial s}\right)^{-1}. \tag{13}$$

With calculating the quantity

$$\begin{aligned} \frac{\partial \eta}{\partial s} &= \ln 2 + \ln\left(\sqrt{4-3s^2}-1\right) - \ln\left(4+3s-\sqrt{4-3s^2}\right) \\ &\quad - \left[\frac{3s\left(\sqrt{4-3s^2}+s\right)}{(4+3s)\sqrt{4-3s^2}-(4-3s^2)} + \frac{3s(s-1)}{4-3s^2-\sqrt{4-3s^2}}\right] \\ &= \ln 2 + \ln\left(\sqrt{4-3s^2}-1\right) - \ln\left(4+3s-\sqrt{4-3s^2}\right), \end{aligned} \tag{14}$$

one can solve the temperature, which reads

$$T = \frac{\epsilon}{k_{\rm B}}\left[\ln\frac{2(1-s)}{\left(s+\sqrt{4-3s^2}\right)}\right]^{-1}, \qquad s = \frac{E}{N\epsilon}\,. \tag{15}$$

In the reduced coordinate, one can introduce a sign $\tilde{\beta} \equiv \beta\epsilon = \frac{\epsilon}{k_{\rm B}T}$. In the micro-canonical ensemble system, Eq. (15) turns into

$$\tilde{\beta}\left(\tilde{E}\right) = \ln\frac{2\left(1-\tilde{E}\right)}{\left(\tilde{E}+\sqrt{4-3\tilde{E}^2}\right)}\,. \tag{16}$$

One can notice that when $s \to 0$, $\frac{\partial \eta}{\partial s} = (-1-1+1) \times \frac{3}{2}s + O(s^2) = -\frac{3}{2}s + O(s^2)$, $E = -\frac{2N\epsilon^2}{3k_{\rm B}T}$. Thus, $T = -\frac{2N\epsilon^2}{3k_{\rm B}E}$. It means that there is a negative temperature in the magnetic system. However, the specific heat $C$, which equals $\frac{2N\epsilon^2}{9k_{\rm B}T^2}$, is still positive.

## 3. Comparison with the canonical ensemble method

In the canonical ensemble form, for the uncoupled system, the partition function reads

$$Z = \frac{1}{N!} Q_1^N \,. \tag{17}$$

Here, the one-particle partition function $Q_1 = 1 + 2\cosh(\beta\epsilon)$. The free energy $F = k_{\rm B}T \ln Z \equiv \frac{\ln Z}{\beta} = NT\{\ln N - 1 - \ln[1 + 2\cosh(\beta\epsilon)]\}$ . The energy reads

$$E = -\frac{2N\epsilon \sinh(\beta\epsilon)}{1 + 2\cosh(\beta\epsilon)} \,, \tag{18}$$

and the entropy is

$$S = N\left\{\ln\left[1 + 2\cosh(\beta\epsilon)\right] - \frac{2\beta\epsilon \sinh(\beta\epsilon)}{1 + 2\cosh(\beta\epsilon)} - \ln N + 1\right\} . \tag{19}$$

When $\beta \to 0$ , $E = -\frac{2N\epsilon^2}{3k_{\rm B}T}$. The result is the same as the one solved by the micro-canonical ensemble method.

In the canonical ensemble system, $\tilde{E}(\tilde{\beta})$ reads

$$\tilde{E} = -\frac{2\sinh\left(\tilde{\beta}\right)}{1 + 2\cosh\left(\tilde{\beta}\right)} \,. \tag{20}$$

The comparison between two methods is showed in Fig. 1. Equations (16) and (20) are located on the same curve.

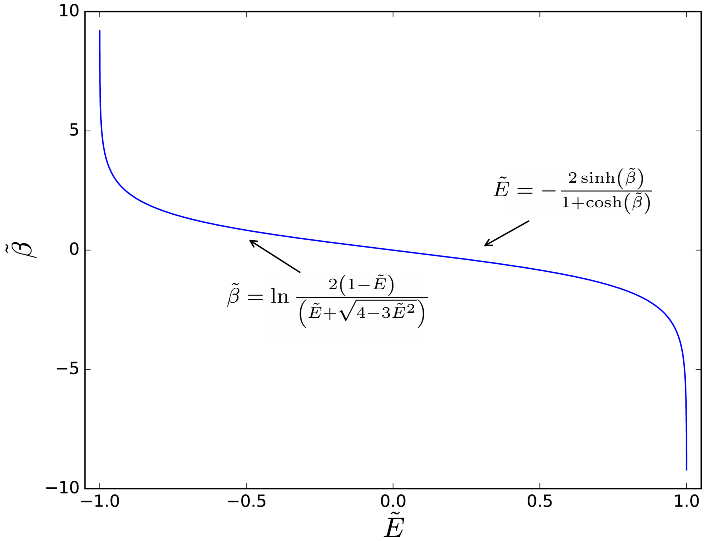


Fig. 1. The comparison between the micro-canonical ensemble and the canonical ensemble.

## 4. Conclusion and discussion

We find an apparently difficult but feasible way to calculate the entropy and temperature of the three-level system using the MCE method. The approximation seems rough but effective. The MCE method has a natural advantage over the CE method in coupled systems where one has to make some perturbation near the energy $E$ or the occupation numbers of the different level $x_i$. This work will set the first step to study interacting multi-level systems.

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