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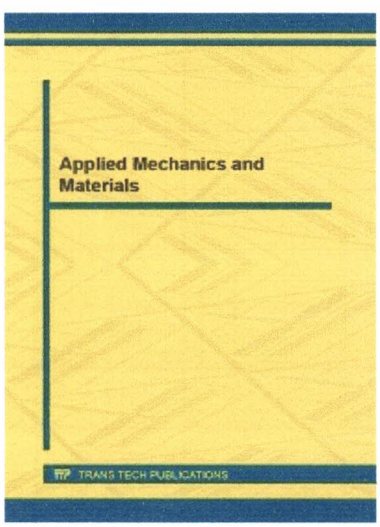

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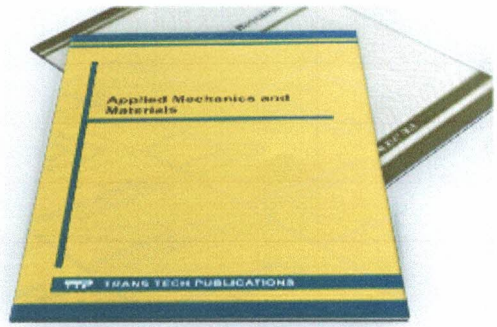

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Preface

In this volume collected articles presented at Uttaradit Rajabhat University International Conference on Science and Technology 2018 (URUICST 2018. August 2-3, 2018, Uttaradit Thailand). The main topics of issue are technologies in the food processing and agriculture, pharmacology and biotechnologies, technologies for production of renewable energy, advanced materials and chemical technologies in the environmental engineering, designing in mechanical engineering and information technologies.

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Applied Mechanics and Materials
ISSN: 1662-7482, Vol. 886, pp 194-200
doi:10.4028/www.scientific.net/AMM.886.194

Submitted: 2018-05-26
Revised: 2018-08-07
Accepted: 2018-08-29
Online: 2019-01-04

Evaluation of Specific Heat Capacity and Entropy of Particle Bound Harmonics Oscillator Cosine Asymmetric Potential by Partition Function

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Keywords: partition function, specific heat capacity, entropy, harmonics oscillator cosine asymmetric potential

Abstract. In this research, a fundamental quantum mechanics and statistical mechanic bound-state problem of harmonics oscillator cosine asymmetric was considered by using partition function method. From the study, it found that the internal energy, the entropy and the specific heat capacity of particle vibration bound-state under harmonics oscillator cosine asymmetric potential were increased as the increasing of the parameters of μ, η, and β. While an increasing of parameter α affected to the decreasing of the entropy and the heat capacity. In addition, the increasing values of the entropy and the specific heat capacity value were depended on the decreasing of the parameter α value.

Introduction

Until now, we have described the macroscopic properties of matter phenomenologically with the aid of equations of state which had been derived empirically. For thermodynamics it is no importance, in this connection, how a certain equation of state come about. We have already seen that many quantities of state and equation state (ideal gas, van der Waals gas)[1,4] can be very well understood with the aid of microscopic considerations. The essential superiority of statistical mechanics however, will not become apparent until the modern formulation of canonical distribution and an ensemble defined by this distribution is called a canonical ensemble. The purpose of this paper, we will evaluate the partition function as a function of temperature, internal energy, entropy, specific heat capacity, enthalpy, free energy and standard deviation. The scheme of the article is as follows. In section (2) we wrote the gamma function basic evaluation of integral Gaussian odd and even function. In section (3) we presented the evaluation of the partition function, the entropy, specific heat capacity of particle bound state in harmonics oscillator cosine asymmetric potential. In section (4) contains our conclusions.

Gamma Function $\left(\Gamma\left(n\right)\right)$

We start with the gamma function, which is identical with the factorial function (n-1)! and definition as the integral form

$$\Gamma(n) \equiv (n-1)! = \int_0^\infty e^{-x} x^{n-1} dx \; ; \; n > 0 \tag{1}$$

Substituting $x = ay^2$ into eq. (1) takes the form

$$\Gamma(n) = 2a^n \int_0^\infty e^{-ay^2} y^{2n-1} dy \; ; n > 0 \tag{2}$$

Thus, we obtained another closely which related to the integral, namely

$$\int_{-\infty}^{\infty} e^{-ay^2} y^n dy = \begin{cases} 0 & \text{for } n = \text{odd intrger} \\ 2I_n, & \text{for } n = \text{even intrger.} \end{cases} \tag{3}$$

The partition function of particle bound state in potential of $V(q) = \alpha q^2 + \beta q^3 + \mu \cos(\eta q^2)$

In the partition function of particle bound state in potential asymmetric. Consideration as we defined that the μ, η, β and α were parameter of the harmonics oscillator cosine asymmetric potential respectively. It was assumed that identical the masses were present in all regions of the structure. The harmonics oscillator cosine asymmetric potential $V(q) = \alpha q^2 + \beta q^3 + \mu \cos(\eta q^2)$ diagram were sketched as show in fig. (1) [5].

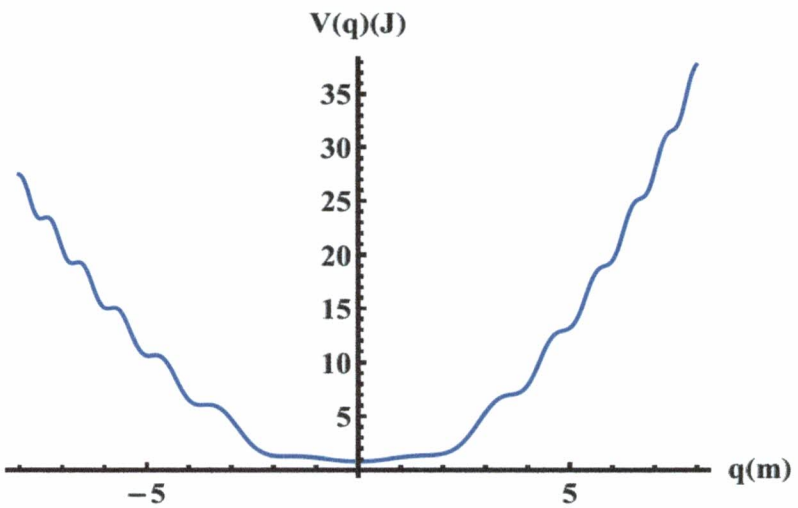

Figure 1 The harmonics oscillator cosine asymmetric potential energy for vibration of a particle bound-state[7]. The unit of distance is the meters.

To solve the problem, it was first necessary to solve the partition function in all regions [2,4,6]. Then, the part of the partition function of an oscillator originating from the potential $V(q)$ was written as this

$$Z = \int_{-\infty}^{\infty} e^{-\frac{V(q)}{k_\beta T}} dq \, . \tag{4}$$

Substituting the potential $V(q)$ into equation (4), we obtain

$$Z = \int_{-\infty}^{\infty} e^{-\frac{\alpha q^2}{k_\beta T}} e^{-\frac{\left(\beta q^3 + \mu \cos(\eta q^2)\right)}{k_\beta T}} dq \, . \tag{5}$$

Since coefficients μ, η, β were positive constant small, the integral was largely determined by the first exponential function, which is appreciable only in the range $q^2 \leq \frac{k_\beta T}{\alpha}$ [2,4,6]. Therefore, the second exponential function factor in equation (5) reflected approximation order in the expansion potential

$$Z(T)=\int_{-\infty}^{\infty} e^{-\frac{\alpha q^2}{k_\beta T}}\left(e^{-\frac{\mu}{k_\beta T}}-\left(\frac{\beta e^{-\frac{\mu}{k_\beta T}}}{k_\beta T}q^3\right)+\left(\frac{\mu\eta^2 e^{-\frac{\mu}{k_\beta T}}}{2k_\beta T}q^4\right)+\left(\frac{\beta^2 e^{-\frac{\mu}{k_\beta T}}}{2\left(k_\beta T\right)^2}q^6\right)\right.$$
$$\left.-\left(\frac{\mu\eta^2\beta e^{-\frac{\mu}{k_\beta T}}}{2\left(k_\beta T\right)^2}q^7\right)+\left(\frac{\mu\eta^4\left(k_\beta T-3\mu\right)e^{-\frac{\mu}{k_\beta T}}}{24\left(k_\beta T\right)^2}q^8\right)-\left(\frac{\beta^2 e^{-\frac{\mu}{k_\beta T}}}{6\left(k_\beta T\right)^3}q^9\right)+\left(\frac{\mu\eta^2\beta^2 e^{-\frac{\mu}{k_\beta T}}}{4\left(k_\beta T\right)^3}q^{10}\right)+\cdots\right)dq. \tag{6}$$

By using the relationship of the integral gamma function from equation(3). Therefore the partition function of an oscillator $Z(T)$ could be expressed that

$$Z(T)=e^{-\frac{\mu}{k_\beta T}}\sqrt{\frac{\pi k_\beta T}{\alpha}}\left\{1+\left(\frac{3\mu\eta^2}{8\alpha^2}\left(k_\beta T\right)\right)-\left(\left(\frac{315\mu^2\eta^4}{384\alpha^4}-\frac{945\mu\beta^2\eta^2}{128\alpha^5}\right)\left(k_\beta T\right)^2\right)\right.$$
$$\left.+\left(\frac{105\mu\eta^4}{384\alpha^4}\left(k_\beta T\right)^3\right)+\cdots\right\}. \tag{7}$$

From partition function [5] is defined in equation (7) and the results of calculating results which derived from the equation have shown in figure (2).

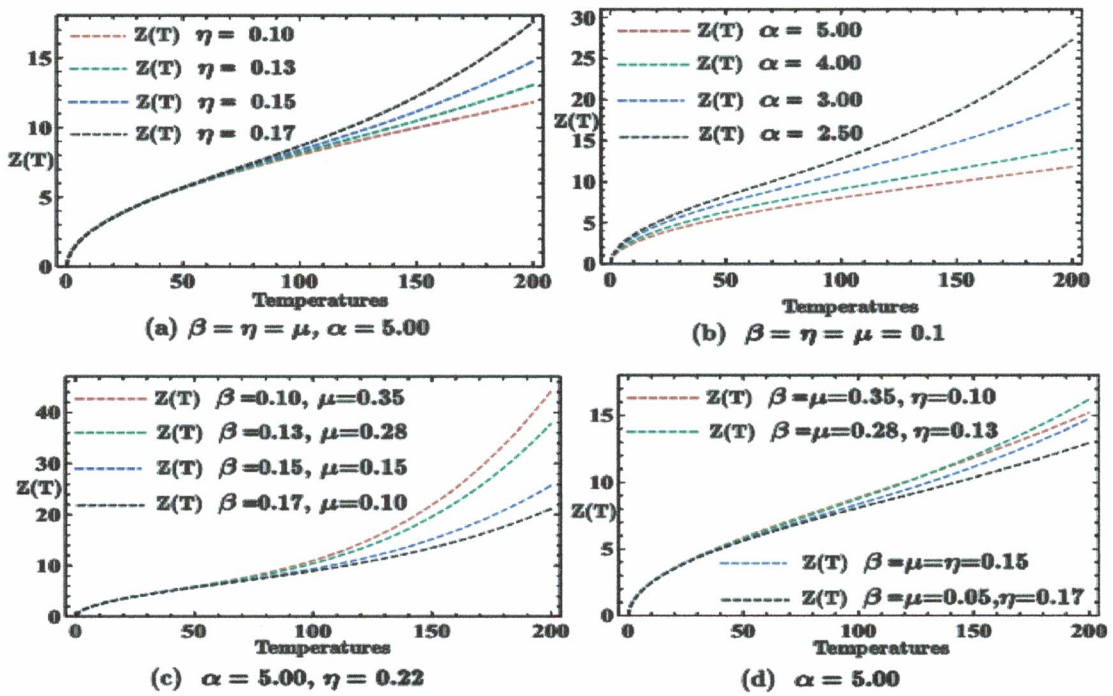

Figure 2 Illustration the partition function of particle bound-state under potential system.

The thermodynamic internal-energy $U(T)$, entropy $S(T)$, could be determined from the microscopic physics of statistical mechanics. The macroscopic work done by the system dW, and displacement, it found that from of the average energy as $dW=\left(\beta_t^{-1}\right)\frac{\partial}{\partial q^2}\left(\ln\left(Z(T)\right)\right)dq$ [5]. With the first law of thermodynamics $dQ=dW+dU$. From the second law of thermodynamics, dS=dQ/T and the definition of $\beta_t=\left(k_\beta T\right)^{-1}$, the right-hand side of the above equation could be rewritten in terms of the entropy as

$$S(T)=k_\beta \ln\left(Z(T)\right)+\frac{U(T)}{T} \tag{8}$$

When taking the logarithm in equation (7) yields

$$\ln\left(Z(T)\right)=-\frac{\mu}{k_\beta T}+\frac{1}{2}\ln\left(\frac{\pi k_\beta T}{\alpha}\right)+\ln\left\{1+\left(\left(\frac{3\mu\eta^2}{8\alpha^2}+\frac{15\beta^2}{16\alpha^3}\right)\left(k_\beta T\right)\right)-\left(\left(\frac{315\mu^2\eta^4}{384\alpha^4}-\frac{945\mu\beta^2\eta^2}{128\alpha^5}\right)\left(k_\beta T\right)^2\right)+\left(\frac{105\mu\eta^4}{384\alpha^4}\left(k_\beta T\right)^3\right)+\cdots\right\} \tag{9}$$

We can easily calculate the mean value of the internal energy per oscillator from the partition function $Z(T)$ by noting the following relationships: $U(T)=k_\beta T^2\frac{\partial}{\partial T}\ln\left(Z(T)\right)$ therefore the mean value of the internal energy per oscillator of a single-particle bound-state under harmonics oscillator cosine asymmetric potential system could be found from differentiation of the logarithm of partition function with respect to temperature, we obtain

$$U(T)=\mu+\frac{k_\beta T}{2}+\left(\left(\frac{3\mu\eta^2}{8\alpha^2}+\frac{15\beta^2}{16\alpha^3}\right)\left(k_\beta T\right)^2\right)-\left(\left(\frac{630\mu^2\eta^4}{384\alpha^4}-\frac{945\mu\beta^2\eta^2}{128\alpha^5}\right)\left(k_\beta T\right)^3\right)+\left(\frac{315\mu\eta^4}{384\alpha^4}\left(k_\beta T\right)^4\right)+\cdots \tag{10}$$

The mean value of the internal energy per oscillator $U(T)$ as a temperature dependent and depend on the parameter μ, η, β and α showed in equation (10). As substituting equation (10) into equation (8), we can rewrite the entropy of the potential $V(q)=\alpha q^2+\beta q^3+\mu\cos\left(\eta q^2\right)$ completely in terms of temperature as

$$S(T)=\frac{k_\beta}{2}\ln\left(\frac{\pi k_\beta T}{\alpha}\right)+k_\beta\ln\left(1+\left(\left(\frac{3\mu\eta^2}{8\alpha^2}+\frac{15\beta^2}{16\alpha^3}\right)\left(k_\beta T\right)\right)-\left(\left(\frac{315\mu^2\eta^4}{384\alpha^4}-\frac{945\mu\beta^2\eta^2}{128\alpha^5}\right)\left(k_\beta T\right)^2\right)+\left(\frac{105\mu\eta^4}{384\alpha^4}\left(k_\beta T\right)^3\right)\right)+\frac{k_\beta}{2}+\left(\left(\frac{3\mu\eta^2}{8\alpha^2}+\frac{15\beta^2}{16\alpha^3}\right)\left(k_\beta^2 T\right)\right)-\left(\left(\frac{630\mu^2\eta^4}{384\alpha^4}-\frac{945\mu\beta^2\eta^2}{128\alpha^5}\right)\left(k_\beta^3 T^2\right)\right)+\left(\frac{315\mu\eta^4}{384\alpha^4}\left(k_\beta^4 T^3\right)\right)+\cdots \tag{10a}$$

The entropy for the particle oscillate in the potential $V(q)=\alpha q^2+\beta q^3+\mu\cos\left(\eta q^2\right)$ system was plotted as a function of temperature as shown in figure (3).

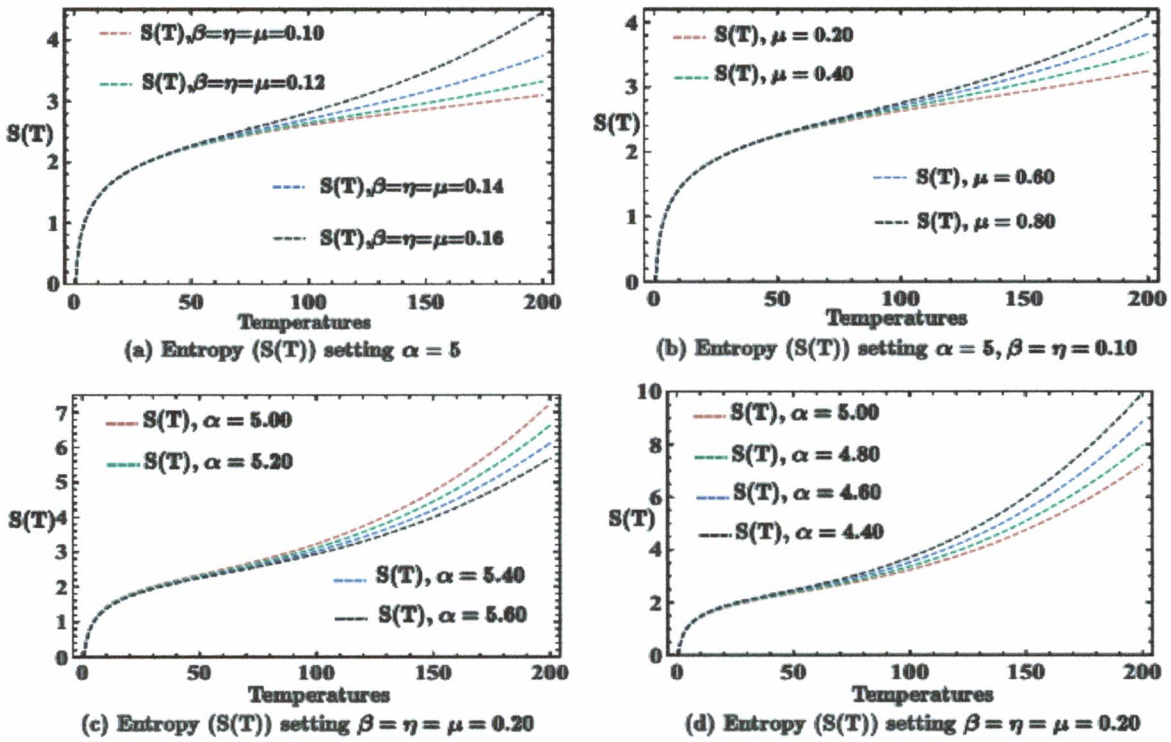

Figure 3 Schematic representation for behavior of the entropy for the particle vibrational bound-state under potential system.

The entropy per oscillator $S(T)$ increase exponentially which depend on the parameter μ, η, β and α .Accordingly, the contribution to the specific heat capacity per oscillation expressed by

$$C_V(T)=\frac{\partial}{\partial T}U(T)=\frac{k_\beta}{2}+\left(\left(\frac{3\mu\eta^2}{8\alpha^2}+\frac{15\beta^2}{16\alpha^3}\right)\left(2k_\beta^2T\right)\right) -\left(\left(\frac{630\mu^2\eta^4}{384\alpha^4}-\frac{945\mu\beta^2\eta^2}{64\alpha^5}\right)\left(3k_\beta^3T^2\right)\right)+\left(\frac{315\mu\eta^4}{96\alpha^4}\left(k_\beta^4T^3\right)\right)+\cdots \tag{11}$$

The specific heat capacity per oscillation $C_V(T)$ as a function of temperature depend on the parameter μ, η, β and α show in the figure (4).

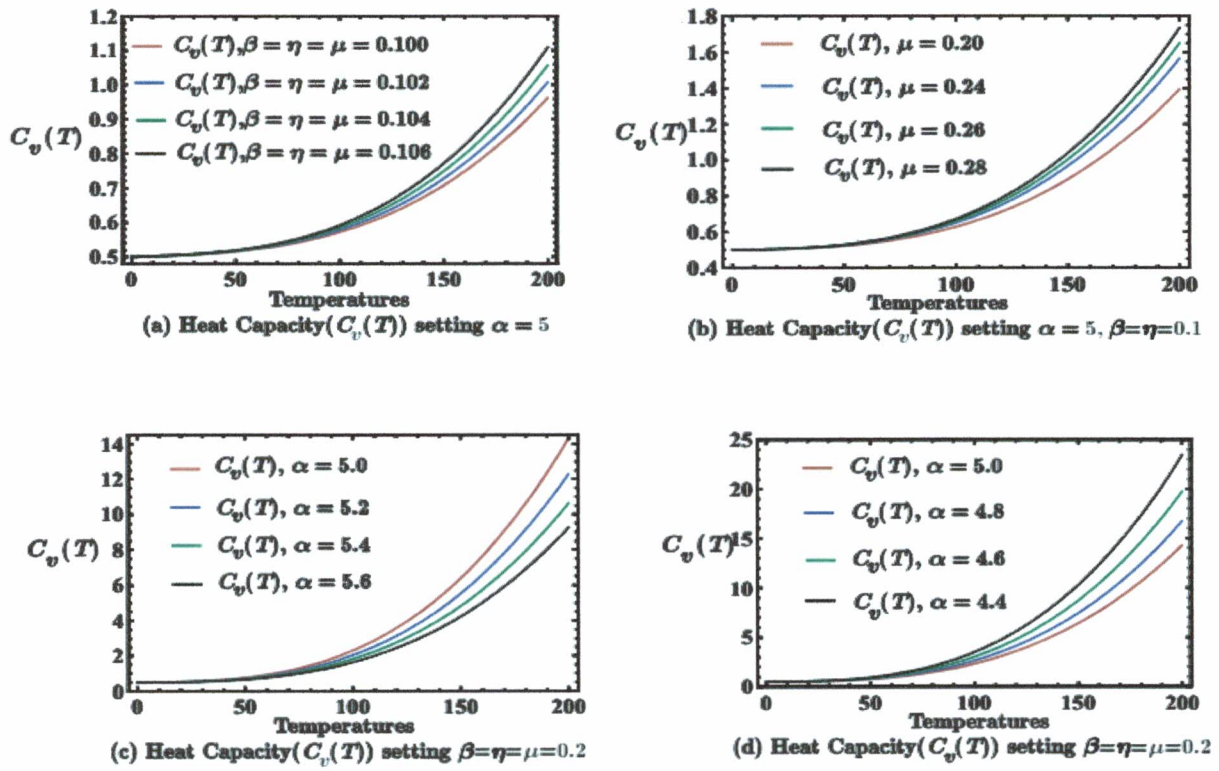

Figure 4 Illustration the specific heat capacity of particle bound-state under potential system.

Discussion and Conclusion

This work, we present the partition function method to obtain the specific heat capacity of particle vibration bound-state under harmonics oscillator cosine asymmetric potential. The results show that the magnitude of the partition function, the entropy and the specific heat capacity of particle vibration bound-state under harmonics oscillator cosine asymmetric potential vary according to the parameters μ, η, β and α, respectively. If the value of each parameter μ,η, β is increased, then the entropy, the specific heat capacity of particle vibration bound-state under harmonics oscillator cosine asymmetric potential have increased. While the values of the α parameter are increased, the entropy, the specific heat capacity of particle vibration bound-state under harmonics oscillator cosine asymmetric potential have decreased. Moreover, we find that as the values of the α parameter are decreased, the entropy, the specific heat capacity of particle vibration bound-state under harmonics oscillator cosine asymmetric potential have increased.
Mention to figure 2(a), when we increase η parameter positive constant from 0.10 to 0.17. It will affect the partition function in the harmonics oscillator cosine asymmetric potential energy to be increased. Mention to figure 2(b), when we decrease α parameter positive constant from 5.00 to 2.50. It will affect the partition function in the harmonics oscillator cosine asymmetric potential energy to be increased. Mention to figure 3(a,b), when we increase μ, η, β parameter positive constant from 0.10 to 0.16 and 0.2 to 0.8. It will affect behavior of the entropy in the harmonics oscillator cosine asymmetric potential energy to be increased.

Acknowledgements

Artit Hutem and Piyarut Moonsri would like to thank the Phetchabun Rajabhat University,Physics for partial support.

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