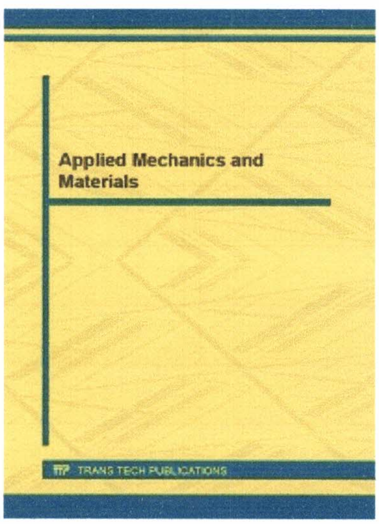
Periodicals

Applied Mechanics and Materials

ISSN: 1662-7482



About:

"Applied Mechanics and Materials" is a peer-reviewed journal which specializes in the publication of proceedings of international scientific conferences, workshops and symposia as well as special volumes on topics of contemporary interest in all areas which are related to:

1) Research and design of mechanical systems, machines and mechanisms;
2) Materials engineering and technologies for manufacturing and processing;
3) Systems of automation and control in the areas of industrial production;
4) Advanced branches of mechanical engineering such as mechatronics, computer engineering and robotics.

"Applied Mechanics and Materials" publishes only complete volumes on given topics, proceedings and complete special topic volumes. We do not publish stand-alone papers by individual authors.

Authors retain the right to publish an extended, significantly updated version in another periodical.

All published materials are archived with PORTICO (http://www.portico.org/digital-preservation/who-participates-in-portico/participating-publishers/transtech) and CLOCKSS (https://www.clockss.org/clockss/Participating_Publishers).

Authors can share research paper via KUDOS platform to help broaden your audience. Share your work via scholarly collaboration networks (like ResearchGate, Academia.edu and Mendeley) in a fully copyrightcompliant way using The Kudos Shareable PDF

Abstracted/Indexed in:
SCImago Journal & Country Rank (SJR) www.scimagojr.com.
Inspec (IET, Institution of Engineering Technology) www.theiet.org.
Chemical Abstracts Service (CAS) www.cas.org.
Google Scholar scholar.google.com.
NASA Astrophysics Data System (ADS) http://www.adsabs.harvard.edu/.
Cambridge Scientific Abstracts (CSA) www.csa.com.
ProQuest www.proquest.com.
Ulrichsweb www.proquest.com/products-services/Ulrichsweb.html.
EBSCOhost Research Databases www.ebscohost.com/.
CiteSeerX citeseerx.ist.psu.edu.
Zetoc zetoc.jisc.ac.uk.
Index Copernicus Journals Master List www.indexcopernicus.com.
WorldCat (OCLC) www.worldcat.org.
ISSN print 1660-9336 ISSN cd 2297-8941 ISSN web 1662-7482

Additional Information:

Please ask for additional information: amm@scientific.net (mailto:amm@scientific.net)

Subscription

Irregular: approx. 20-30 volumes per year.

Rates 2019 for:
- Web 2019: EUR 1'154,-,
- Web 'All BackVolumes 2018-till Vol. 1': EUR 44'000,-,
- Print or CD 2019 (+free WEB): EUR 2'946,- (incl. Postage)

Share:

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.

Committees

Advisory Board

Ruangdet	Wongla	-Uttaradit Rajabhat University, Thailand
Chanboon	Sathiwiriyawong	-King Mongkut's Institute of Technology Ladkrabang, Thailand
Lung-Jen	Wang	-National Pingtung University, Taiwan
Somyot	Plubtieng	-Naresuan University, Thailand
Charles Christopher	Sorrell	-NewSouthwales, Australia
Peter C.	Angelletti	-University of Nebraska, Lincoln, USA
Musumari Masika	Patou	-University School of Public Health, Japan
Michael	Hamlin	- Lincoln University, Newzeland
Jun	Chen	- University of Wollonggong, Australia
Ilhan M.	Cagirgan	- Akdeniz University, Turkey
Stanley R.	Ingman	- University of North Texas, USA
Andrew	Minett	- University of Sydney, Australia
Tharapong	Vitidsant	-Chulalongkorn University, Thailand

Local Organizing Committee

Chair:	Ruangdet Wongla, Uttaradit Rajabhat University, Thailand
Co-Chair:	Supavinee Sattayaporn, Uttaradit Rajabhat University, Thailand
General Secretary:	Kittiwan Junrith, Uttaradit Rajabhat University, Thailand
	Porntippa Pinyapong, Uttaradit Rajabhat University, Thailand
	Jiraporn Nikomtat, Uttaradit Rajabhat University, Thailand
	Kanokwan Kunyamee, Uttaradit Rajabhat University, Thailand
Committee Members:	Napaporn Junsee, Uttaradit Rajabhat University, Thailand
	Siriwadee Promnoi, Uttaradit Rajabhat University, Thailand
	Natkrita Boonprakob, Uttaradit Rajabhat University, Thailand
	Chattanong Podong, Uttaradit Rajabhat University, Thailand
	Surapon Chumklin, Uttaradit Rajabhat University, Thailand
	Chanida Ruangsiriwattanakul, Uttaradit Rajabhat University, Thailand
	Thitiporn Thiankhanthikun, Uttaradit Rajabhat University, Thailand
	Issara Inchan, Uttaradit Rajabhat University, Thailand
	Nicharee Jaikhumwang, Uttaradit Rajabhat University, Thailand
	Pongsak Onmoy, Uttaradit Rajabhat University, Thailand
	Worrawut Thuwakum, Uttaradit Rajabhat University, Thailand
	Pornthep Junpeng, Uttaradit Rajabhat University, Thailand
	Saranyoo Ruanjan, Uttaradit Rajabhat University, Thailand
	Photjanee Inchan, Uttaradit Rajabhat University, Thailand

Main Themes

URU International Conference on Science and Technology 2018

Volume 886
doi: https://doi.org/10.4028/www.scientific.net/AMM.886

Search

< 1 2 3 4 >

Paper Title	Page
Adsorption of H_2S Gas by Modified Diatomite and Leonardite Authors: Weerasak Chomkitichai, Panjaporn Sujit, Jiraporn Ketwaraporn, Pusit Pookmanee, Sukon Phanichphant, Pongthep Jansanthea Abstract: This research aimed to modify of diatomite and leonardite for adsorption of hydrogen sulfide (H_2S) gas. The effect of chemical loading on surface modification was ...more	130
Dye Mixtures Degradation by Multi-Phase $BiVO_4$ Photocatalyst Authors: Weerasak Chomkitichai, Jiraporn Pama, Pimchanok Jaiyen, Sila Pano, Jiraporn Ketwaraporn, Pusit Pookmanee, Sukon Phanichphant, Pongthep Jansanthea Abstract: The objective of this research was to prepare multi-phase bismuth vanadate ($BiVO_4$) powder using the solvothermal method to be used as a photocatalyst. In the ...more	138
Synthesis of Indium Sulfide/Zinc Oxide Composites Films and their Photocatalytic Activities Authors: Natkritta Boonprakob, Anchalee Masa-Ad Abstract: Indium sulfide and zinc oxide (In_2S_3-ZnO) films have successfully synthesized by doctor blading method coupling with low temperature precipitation-reflux rout. The	146

investigated. To describe rock properties of the selected outcrops, density,
...more

Main Themes

URU International Conference on Science and Technology 2018

Volume 886
doi: https://doi.org/10.4028/www.scientific.net/AMM.886

Search

< 1 2 3 4

Paper Title	Page
Theory Mathematics and Physics Model Fitting of Kinematic Parameter for Usain Bolt 100 Metres Sprint at Beijing Olympic Games 2008 Authors: Nichapat Thongsit, Yosita Sangnok, Wannee Wannapak, Kan Khoomsab, Surachest Iamsamang, Sirada Sangnok, Jetsadaporn Pakamwang, Artit Hutem Abstract: In this paper, we develop a mathematical and physics model or formula of displacement-time dependent, velocity-time dependent, acceleration-time dependent, ...more	201
Determine the Specific Heat Capacity, the Entropy, and the Standard Deviation of Particle Vibration Bound-State under the Anharmonic Oscillator Asymmetric Potential by Partition Function Method Authors: Metaporn Apiratigosol, Katang Jeeradit, Pattadon Keawpeai, Supaporn Hutem, Artit Hutem, Sanit Suwanwong, Piyarut Moonsri Abstract: In this work, we consider is the single-particle bound-state problem. A single-particle moves in the absence of the anharmonics oscillator asymmetric potential. The ...more	206
Effect of Filler Types on Properties of the Natural Rubber Closed Cell Foam Authors: Ekaroek Phumnok, Jakkrit Boonphang, Orrachorn Bourkaew Abstract: In this research, effects of filler types and their loading on properties of the	213

Gmail

Metaporn Apiratigosol <metapornsol666@gmail.com>

Your paper has been accepted for publication in International Conference on Science and Technology 2018

1 message

International Conference on Science a... <9783035714142@scientific.net> Wed, Aug 29, 2018 at 9:40 AM
Reply-To: "International Conference on Science a..." <9783035714142@scientific.net>
To: Metaporn Apiratigosol <metapornsol666@gmail.com>

Dear Metaporn Apiratigosol,

Your paper «Determine the Specific Heat Capacity, the Entropy, and the Standard Deviation of Particle Vibration Bound-State under the Anharmonic Oscillator Asymmetric Potential by Partition Function Method» has been accepted for further quality check in order to be published* in the «International Conference on Science and Technology 2018» . Although no further action is required, you can verify the status of your manuscript by logging in to the publisher's website :

Please go to https://www.scientific.net/ and log in using the credentials below.
Username : metapornsol666@gmail.com
Password : QCjxf237

After you login please select « Participant » near the top of the screen.

If any further changes to your manuscript become necessary you must notify and obtain permission of an Editor via E-mail PRIOR to uploading a new version. Thank you very much.

Best regards,
Kittiwan Junrith
uruicst@uru.ac.th

====================

Uttaradit Rajabhat University
International Conference on Science and Technology 2018

====================

**Before the publication all of the manuscripts accepted by editors undergo an additional internal quality check. They are verified for the absence of the plagiarism and redundant publication. The accepted manuscripts which do not pass this quality check are rejected from the publication in the journal.*

Applied Mechanics and Materials
ISSN: 1662-7482, Vol. 886, pp 206-212
doi:10.4028/www.scientific.net/AMM.886.206

Submitted: 2018-05-27
Revised: 2018-08-07
Accepted: 2018-08-29
Online: 2019-01-04

Determine the Specific Heat Capacity, the Entropy, and the Standard Deviation of Particle Vibration Bound-State under the Anharmonic Oscillator Asymmetric Potential by Partition Function Method

Metaporn Apiratigosol[1,a], Katang Jeeradit[1,b], Pattadon Keawpeai[1,c]
Supaporn Hutem[1,c], Artit Hutem[2,f*], Sanit Suwanwong[2,e], Piyarut Moonsri[3,d]

[1]Wittayanukulnaree School, Ni-Muang Sub District, Muang District, Phetchabun, Thailand 67000

[2]Physics Division, Faculty of Science and Technology, Phetchabun Rajabhat University, Phetchabun, Thailand 67000

[3]Chemistry Division, Faculty of Science and Technology, Phetchabun Rajabhat University, Phetchabun, Thailand 67000

[a]cardphone43@gmail.com, [b]katangjee@hotmail.com, [c]S.hutem@yahoo.com, [d]Piyarutto@hotmail.com, [e]sanit.suw@gmail.com [*f]artithutemdee@gmail.com

*Corresponding author: Fax: 056-717-123, Mobile: 086-9909536

Keywords: partition function, specific heat capacity, entropy, standard-deviation, anharmonics oscillator asymmetric potential

Abstract. In this work, we consider is the single-particle bound-state problem. A single-particle moves in the absence of the anharmonics oscillator asymmetric potential. The bound-state problem then is to solve the partition function for single-particle in the presence of anharmonics oscillator asymmetric potential. The factor second exponential function of partition function of particle bound in the anharmonics oscillator asymmetric potential can also be expanded in power series of the temperature and parameter b, c, d and x is the position of single-particle bound-state problem and using the integrate Gaussian. The purpose of this works, we will compute the partition function as a function of temperature, entropy, specific heat capacity and standard deviation which depend on the c,d parameter and frequency (f).

Introduction

In general, the macroscopic world consists of many particles simultaneously interacting with one another. Currently, it had shown the direct interaction algorithm (DIA) for approximating the canonical partition function Z_N in N^2 operations and the DIA was used to compute equilibrium properties for the isotropic 2D Ising model, and the accuracy of the DIA was compared to that of basic Metropolis Monte Carlo method [3]. And the numerically studied the standard canonical sampling of phase space to directly compute the partition function and heat capacity [4]. In addition a method for calculating partition function taking into account anharmonic contributions for system involving both small-amplitude vibration and hindered rotations was present by Skouteris et. al.[6]. The purpose of this works, we will compute 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 write the basic evaluation of integral Gaussian odd and even function. In section (3) we illustrate evaluation of the partition function, internal energy, entropy, specific heat capacity, enthalpy, free energy and standard deviation of particle bound state in anharmonics oscillator asymmetric potential. In section (4) contains our conclusions.

Evaluation of Integral

An important example of this method is provided by the evaluation of integral

$$I=\int_{-\infty}^{\infty} e^{-x^2}\,dx \tag{1}$$

Its value may be found by first constructing I^2 , as follow :

$$I^2=\int_{-\infty}^{\infty} e^{-x^2}\,dx\int_{-\infty}^{\infty} e^{-y^2}\,dy=\iint_R e^{-\left(x^2+y^2\right)}dxdy, \tag{2}$$

where the region R is the whole xy-plane. The differential dx dy represents an elementof area in cartesian coordinates, with the domain of integration extending over the entire xy-plane An alternative representation of the last integral can be expressed in plane polar coordinates r, θ. The two coordinate systems are related by $x=r\cos\theta$, $y=r\sin\theta$, The element of area in polar coordinates is given by r dr dθ, so that the double integral becomes

$$I^2=\iint_R e^{-\rho^2}\rho\,d\rho d\phi=\int_0^{2\pi}d\phi\int_0^{\infty}\rho e^{-\rho^2}d\rho=2\pi\left[-\frac{1}{2}e^{-\rho^2}\right]_0^{\infty}=\pi.$$

Therefore the original integral is given by $I=\sqrt{\pi}$. We not, however, that unlike in all the previous examples, the regions of integration R' and R' are both infinite in extent. It is therefore prudent to derive this result more rigorously; this we do by considering the integral

$$\int_{-\infty}^{\infty} e^{-ax^2}dx=\frac{1}{\sqrt{a}}\int_{-\infty}^{\infty} e^{-ay^2}dy=\sqrt{\frac{\pi}{a}}, \tag{3}$$

and integrate gaussian even function

$$\int_{-\infty}^{\infty} x^2e^{-ax^2}dx=-\int_{-\infty}^{\infty}\frac{\partial}{\partial a}e^{-ax^2}dx=-\frac{d}{da}\int_{-\infty}^{\infty} e^{-ax^2}dx=-\frac{d}{da}\sqrt{\frac{\pi}{a}}=\frac{1}{2}\sqrt{\pi}a^{-\frac{3}{2}}, \tag{4}$$

and integrate gaussian odd function

$$\int_{-\infty}^{\infty} x^2e^{-ax^2}dx=0 \tag{5}$$

and integrate gaussian even function

$$\int_{-\infty}^{\infty} x^4e^{-ax^2}dx=-\int_{-\infty}^{\infty}\frac{\partial^2}{\partial a^2}e^{-ax^2}dx=-\frac{d^2}{da^2}\int_{-\infty}^{\infty} e^{-ax^2}dx=\frac{4}{4}\sqrt{\pi}a^{-\frac{5}{2}}, \tag{6}$$

and

$$\int_{-\infty}^{\infty} x^6e^{-ax^2}dx=-\int_{-\infty}^{\infty}\frac{\partial^3}{\partial a^3}e^{-ax^2}dx=\frac{\partial^2}{\partial a^2}\left(-\int_{-\infty}^{\infty} x^2e^{-ax^2}dx\right)=\frac{15}{8}\sqrt{\pi}a^{-\frac{7}{2}}, \tag{7}$$

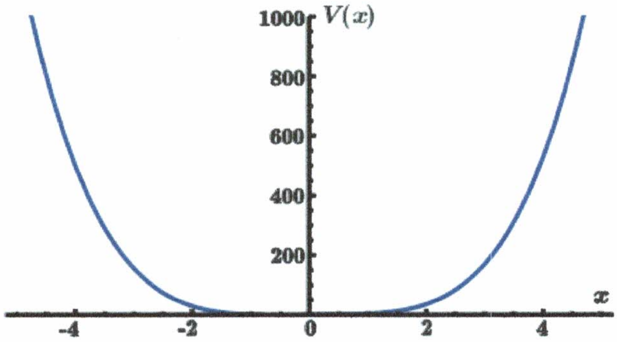


Fig. 1: The anharmonics oscillator asymmetric potential system.

Let us consider a problem to illustrate the use of integrate Gussian function(see eq4-eq7). An interesting work is that of a particle move under the influence of the anharmonics oscillator asymmetric potential in section (3).

Evaluation of the Partition Function of Particle Bound State in Anharmonics Oscillator Asymmetric Potential

In this section, we consider the statistical mechanics behavior of a particle that moves under the influence of the anharmonics oscillator asymmetric potential as

$$V(x)=\frac{1}{2}m\omega^2x^2+bx+cx^3+dx^4 \tag{8}$$

where b, c , and d is parameter positive constant. The problem then is to solve the partition function for a particle in the presence of the anharmonics oscillator asymmetric potential see figure (1). The partition function of particle bound in the anharmonics oscillator asymmetric potential is

$$Z(T)=\int_{-\infty}^{\infty} e^{-\frac{m\omega^2}{2kT}x^2} e^{-\frac{1}{kT}\left(bx+cx^3+dx^4\right)}dx \tag{9}$$

Formally, if we expand the exponential function in a Taylor series about the mininmun:

$$e^{-\frac{1}{kT}\left(bx+cx^3+dx^4\right)}=1-\frac{bx}{kT}+\frac{b^2x^2}{2(kT)^2}-\frac{cx^3}{kT}+\left(\frac{bc}{(kT)^2}-\frac{d}{kT}\right)x^4+\frac{bd}{(kT)^2}x^5+\frac{c^2}{2(kT)^2}x^6+\cdots \tag{10}$$

Since the coefficients b, c , and d are small, the integral is largely determined by the first exponential function, which is appreciable only in the range $x^2 \le 2kT / m\omega^2$. In this range, $cx^3 / kT \le c\sqrt{kT} / \left(m\omega^2 / 2\right)^{\frac{1}{2}} \ll 1$ and $dx^4 / kT \le dkT / \left(m\omega^2 / 2\right)^2 \ll 1$.

Substituting equation (10) and using integrate gaussian of equation (4)-(7) into equation (9), we can rewrite the partition function completely in terms of temperature as

$$Z(T)=\sqrt{\frac{2\pi kT}{m\omega^2}}\left\{1+\frac{b^2}{2mkT\omega^2}+\frac{3bc}{m^2\omega^4}-\frac{12d}{4m^2\omega^4}(kT)+\frac{15c^2}{2m^3\omega^6}(kT)+\frac{105d^2}{2m^4\omega^8}(kT)^2+\cdots\right\} \tag{11}$$

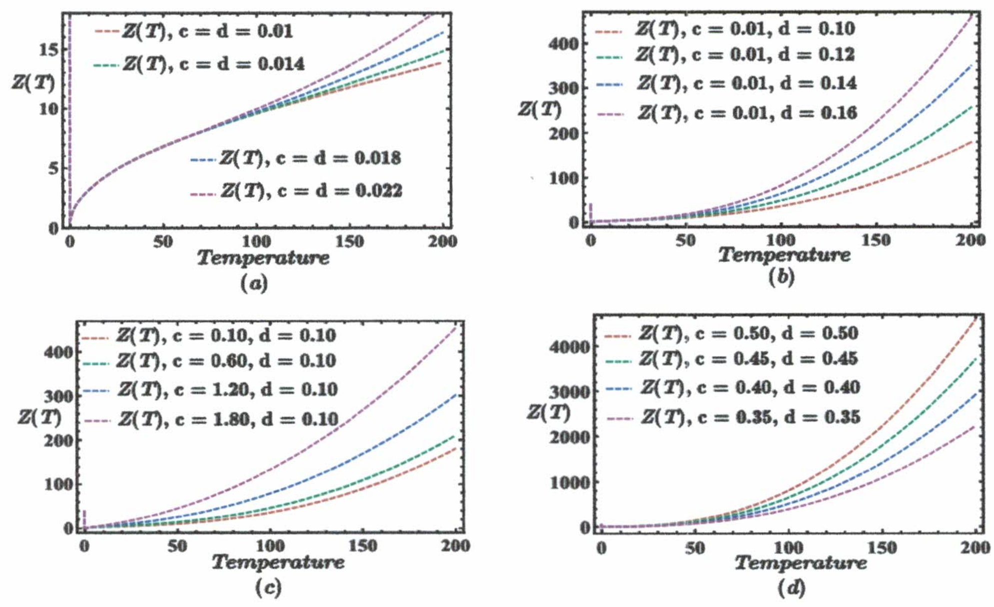


Fig. 2: Partition function as a function of temperature plotted for c and d is parameter. positive constant.

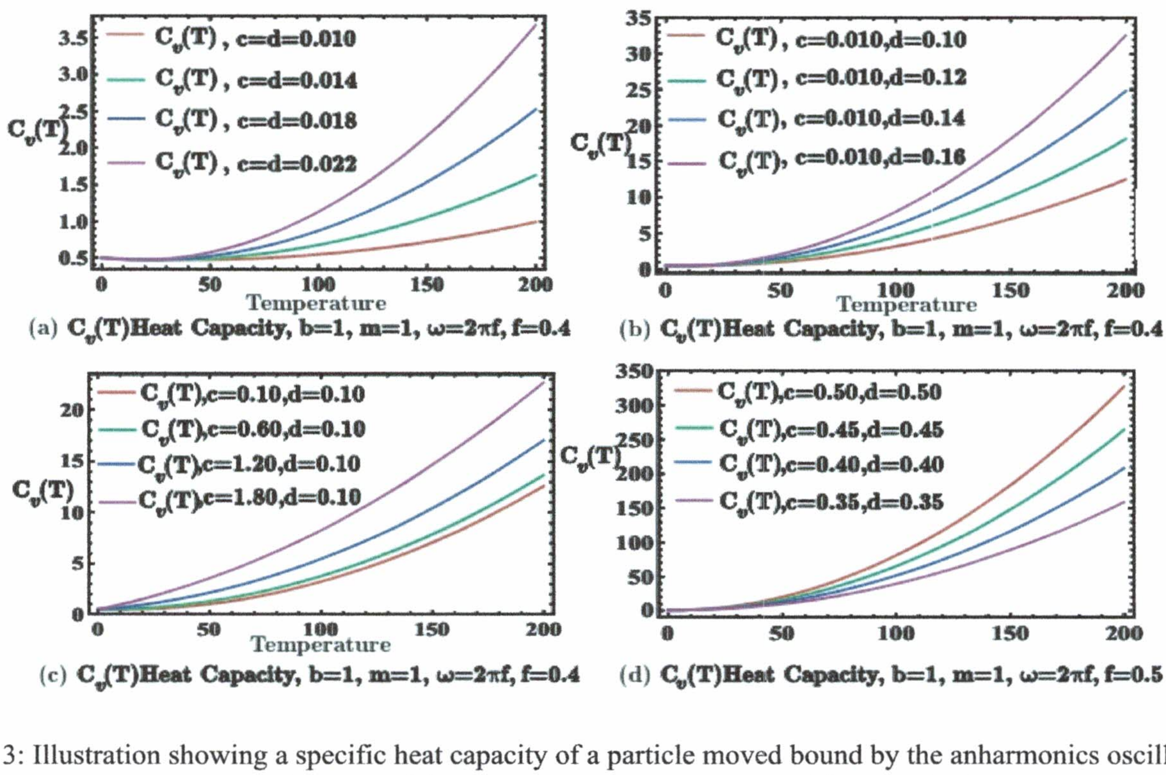
Schematically drawn, the partition function in equation (11) has the shape shown in figure (2). Hence from knowledge of the partition function $Z(T)$, the internal energy per oscillation $U(T)$, the entropy per oscillation $S(T)$, the specific heat capacity per oscillation $C_v(T)$ and the variance of position of particle vibration bound-state under anharmonics oscillator asymmetric potential system can be readily determined. As a result, all the thermodynamics anharmonics oscillator asymmetric potential can then be determined, provided that the macroscopic observable $S(T)$, $C_v(T)$ and the free energy are known as well. Subsequently the result of the classical thermodynamics are recovered from statistical mechanics. The contribution to the temperature dependent internal energy per oscillation is $U(T)=kT^2\frac{\partial}{\partial T}\left(\ln\left(Z(T)\right)\right)$. Taking the logarithm and the derivative yields in the partition function on the equation (11) for the temperature dependent internal energy per oscillation

$$U(T)=kT^2\frac{\partial}{\partial T}\left(\ln\left(Z(T)\right)\right)=kT^2\left(\frac{1}{2}\frac{\partial}{\partial T}\ln\left(\frac{2\pi kT}{m\omega^2}\right)+\frac{\partial}{\partial T}\ln\left(1+\frac{3bc}{m^2\omega^4}+\frac{b^2}{2mkT\omega^2}+\left(\frac{15c^2}{2m^3\omega^6}-\frac{d}{4m^2\omega^4}\right)(kT)+\frac{105d^2}{2m^4\omega^8}(kT)^2\right)\right), \tag{12}$$

We can determine the temperature dependent specific heat capacity from the above by taking the derivative with respect to the temperature

$$C_v(T)=\frac{\partial}{\partial T}U(T)=\frac{k}{2}+2\left(\frac{15c^2}{2m^3\omega^6}-\frac{12d}{4m^2\omega^4}\right)\left(k^2T\right)+\frac{315d^2}{2m^4\omega^8}\left(k^3T^2\right)+\cdots. \tag{13}$$

Schematically sketch, the temperature dependent specific heat capacity in equation (13) has shape illustrate in figure (3). The temperature dependent entropy then defined as



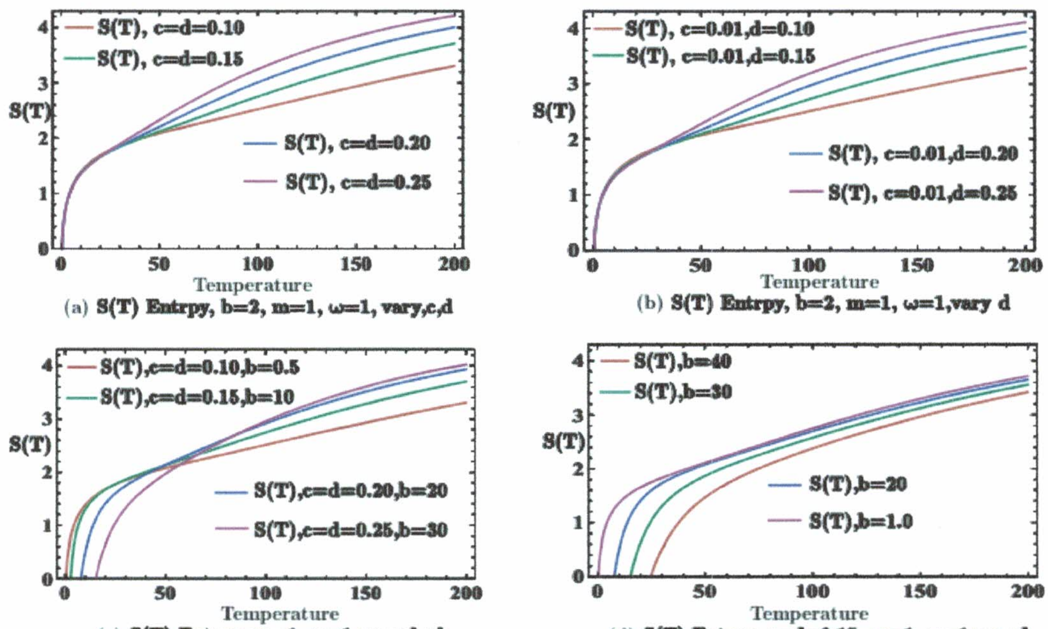
(a) $C_v(T)$Heat Capacity, b=1, m=1, ω=2πf, f=0.4
(b) $C_v(T)$Heat Capacity, b=1, m=1, ω=2πf, f=0.4
(c) $C_v(T)$Heat Capacity, b=1, m=1, ω=2πf, f=0.4
(d) $C_v(T)$Heat Capacity, b=1, m=1, ω=2πf, f=0.5

Fig. 3: Illustration showing a specific heat capacity of a particle moved bound by the anharmonics oscillator asymmetric potential and vary c and d parameter positive constant.

$$S(T)=k\ln\left(Z(T)\right)+\frac{U(T)}{T}$$

$$S(T)=\frac{k}{2}\ln\left(\frac{2\pi kT}{m\omega^2}\right)+k\ln\left(1+\frac{3bc}{m^2\omega^4}+\frac{b^2}{2mkT\omega^2}+\left(\frac{15c^2}{2m^3\omega^6}-\frac{12d}{4m^2\omega^4}\right)(kT)+\frac{105d^2}{2m^4\omega^8}(kT)^2\right)$$

$$+\frac{k}{2}-\frac{b^2}{2mkT\omega^2}+\left(\frac{15c^2}{2m^3\omega^6}-\frac{12d}{4m^2\omega^4}\right)(kT)+\frac{105d^2}{2m^4\omega^8}(kT)^2+\cdots \tag{14}$$



(a) S(T) Entrpy, b=2, m=1, ω=1, vary,c,d

(b) S(T) Entrpy, b=2, m=1, ω=1,vary d

(c) S(T) Entrpy, m=1, ω=1,vary d,c,b

(d) S(T) Entrpy, c=d=0.15, m=1, ω=1,vary b

Fig. 4: Plot of the temperature-dependent entropy for particle move in the anharmonics oscillator asymmetric potential.

Sketch of the temperature dependent entropy for this system are given in figure (4). We can determine the temperature enthalpy from defined as $H(T)=U(T)+PV$ by setting P is the pressure, V is the volume of the anharmonics oscillator asymmetric potential system in $V(x)$

$$H(T)=\frac{kT}{2}-\frac{b^2}{2m\omega^2}+\left(\frac{b^2}{2m^3\omega^6}-\frac{12d^2}{4m^2\omega^4}\right)(kT)^2+\frac{105d^2}{2m^4\omega^8}(kT)^3+PV+\cdots \tag{15}$$

The temperature dependent free energy of Helmholtz potential then defined in the anharmonics oscillator asymmetric potential system as $G(T)=U(T)-TS(T)$

$$G(T)=-\left(\frac{kT}{2}\ln\left(\frac{2\pi kT}{m\omega^2}\right)+kT\ln\left(1+\frac{3bc}{m^2\omega^4}+\frac{b^2}{2m\omega^2kT}+\left(\frac{15c^2}{2m^3\omega^6}-\frac{12d}{4m^2\omega^4}\right)(kT)+\frac{105d^2}{2m^4\omega^8}(kT)^2\right)\right) \tag{16}$$

The enthalpy and the temperature dependent free energy of Helmholtz potential of particle for the anharmonics oscillator asymmetric potential system is given by dependent on the parameter b, c, and d. Now consider the average value of the x coordinate for a single-particle oscillation one-dimensional system in the partition function of equation (11). The x coordinate takes on a continuous range of values, and the probability of observing the particle oscillator between x and $x+dx$ is $e^{-\beta V(x)}/Z(T)$ where β is 1/kT. The summation over the infinitesimal probabilities is equivalent to an integration over the full range of x becomes

$$\langle x\rangle=\frac{1}{Z(T)}\int_{-\infty}^{\infty}xe^{-V(x)/kT}dx \tag{17}$$

Substituting the potential $V(x)$ and using the Taylor series expansion and using equation (3)-(7) into equation (17) result in the average value of position x dependent on temperature

$$\langle x\rangle=\frac{1}{Z(T)}\sqrt{\frac{2\pi kT}{m\omega^2}}\left\{-\frac{b}{m\omega^2}-\frac{3c(kT)}{m^2\omega^4}+\frac{15bd(kT)}{m^3\omega^6}+\frac{105cd(kT)^2}{m^4\omega^8}+\cdots\right\}. \tag{18}$$

The average value $\langle x^2\rangle$ of the position of a particle is given by

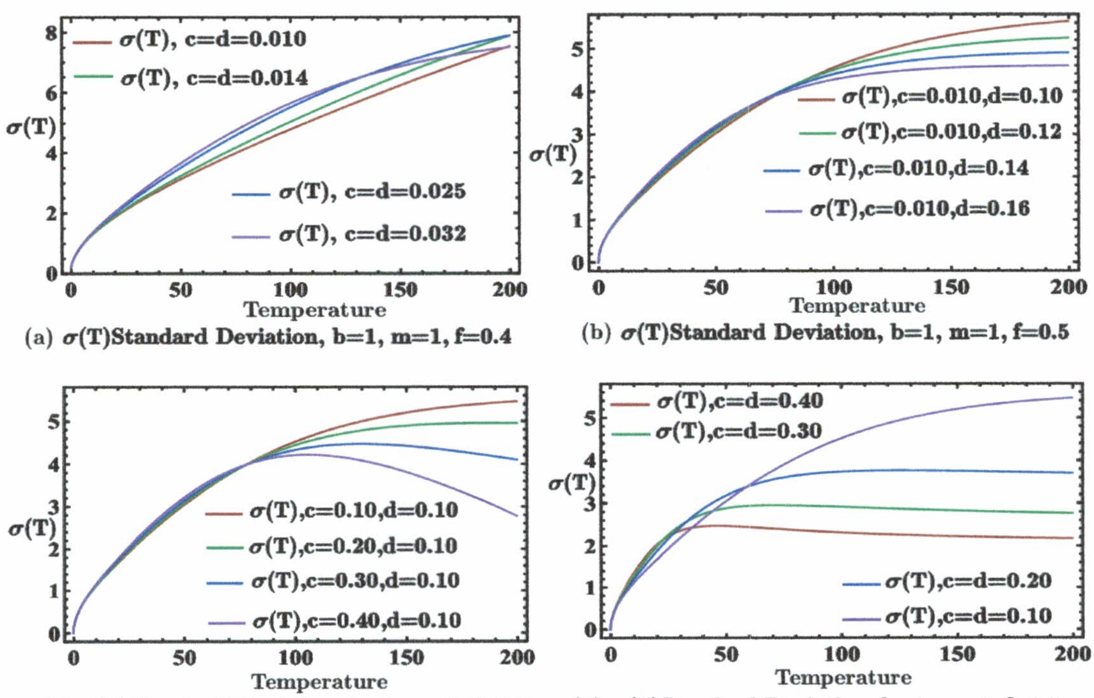
$$\langle x^2\rangle=\frac{1}{Z(T)}\int_{-\infty}^{\infty}x^2e^{-V(x)/kT}dx \tag{19}$$

We again use the potential $V(x)$ and the Taylor series expansion and using equation (3)-(7) into equation (19), we get

$$\langle x^2\rangle=\frac{1}{Z(T)}\sqrt{\frac{2\pi kT}{m\omega^2}}\left\{\frac{3b^2}{2m^2\omega^4}+\left(\frac{1}{m\omega^2}+\frac{15c}{m^3\omega^6}\right)(kT)+\left(\frac{105c^2}{2m^4\omega^8}+\frac{15d}{m^3\omega^6}\right)(kT)^2+\cdots\right\} \tag{20}$$

The standard deviation $\sigma(T)$ of the position of the particle is defined as the root-mean-square deviation $\sigma(T)=\sqrt{\langle x^2\rangle-\langle x\rangle^2}$ of the value of x from the average or the expectation value. Therefore

$$\sigma(T)=\left(\frac{1}{Z(T)}\sqrt{\frac{2\pi kT}{m\omega^2}}\left\{\frac{3b^2}{2m^2\omega^4}+\left(\frac{1}{m\omega^2}+\frac{15c}{m^3\omega^6}\right)(kT)+\left(\frac{105c^2}{2m^4\omega^8}+\frac{15d}{m^3\omega^6}\right)(kT)^2+\cdots\right\}\right.$$
$$\left.-\left(\frac{1}{Z(T)}\sqrt{\frac{2\pi kT}{m\omega^2}}\left\{-\frac{b}{m\omega^2}-\frac{3c(kT)}{m^2\omega^4}+\frac{15bd(kT)}{m^3\omega^6}+\frac{105cd(kT)^2}{m^4\omega^8}+\cdots\right\}\right)^2\right)^{\frac{1}{2}} \tag{21}$$



(a) σ(T)Standard Deviation, b=1, m=1, f=0.4

(b) σ(T)Standard Deviation, b=1, m=1, f=0.5

(c) σ(T)Standard Deviation, b=1, m=1, f=0.5

(d) σ(T)Standard Deviation, b=1, m=1, f=0.5

Fig. 5: Plot of the temperature-dependent standard deviation for particle move in the anharmonics oscillator asymmetric potential.

Discussion and Conclusion

Mention to figure (2), when we increase c and d parameter positive constant from 0.01 to 0.35 and 0.1 to 1.8. It will affect the partition function in the anharmonics oscillator asymmetric potential to be escalated. Mention to figure (3), when we increase c, d parameter positive constant from 0.01 to 0.5. It will affect the specific heat capacity in the anharmonics oscillator asymmetric potential to be increased. Mention to figure (4(a-d)), when we increase c,d parameter positive constant from 0.01 to 40. It will affect the entropy in the anharmonics oscillator asymmetric potential to be escalated. According to figure (5(a)), when we vary c=d parameter positive constant from 0.01 to 0.032. It will affect the standard deviation in potential to be increased $\sigma(T)$=8. Summary, such the partition function, internal energy, specific heat capacity, entropy, enthalpy, free energy and standard deviation which depend on the c,d parameter and frequency (f).

Acknowledgements

Artit Hutem and Piyarut Moonsri would like to thank the Phetchabun Rajabhat University, Physics Division and and Chemistry Division. And also Faculty of Science and Technology, Phetchabun Rajabhat University for partial support.

References

[1] R. Kubo, Statistical Mechanics an Advanced Course with Problems and Solutions, North-Holland Personal Library, 2004, pp.135-158.

[2] Ira N. Levine, Quantum Chemistry, Sixth Edition, Pearson Prentice Hall Education International, 2009, pp.65-96.

[3] R. Anandakrishnan, A Partition Function Approximation Using Elementary Symmetric Functions, Plosone, Volume 7, Issure 12, 2012, pp.e51352.

[4] S. O. Nielsen, Nested sampling in the canonical ensemble: Direct calculation of the partition function from NVT trajectories, J. Chem. Phys., 139, 2013, pp.124104.

[5] A. Hutem and P. Moonsri, Evaluated Excited-State Time-Independent Correlation Function and Eigenfunction of the Harmonics Oscillator Cosine Asymmetric Potential via Numerical Shooting Method, Physics Research International, Volume 2015, Article ID 609495.

[6] D. Skouteris et. al., Methods for Calculating Partition Functions of Molecules Involving Large Amplitude and/or Anharmonic Motions, J. Chem Theory. Comput, 12 , 2016, pp.1011-1018.