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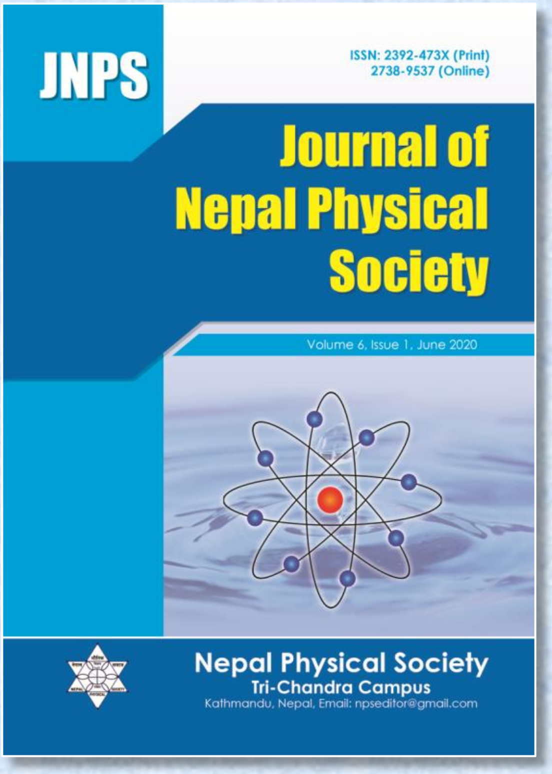

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Path Integral Simulations of Harmonic Oscillator

H. K. Neupane[1, 2] and N. P. Adhikari[2, *]
[1] Amrit Campus, Institute of Science and Technology Tribhuvan University, Kathmandu, Nepal
[2] Central Department of Physics, Institute of Science and Technology Tribhuvan University, Kathmandu, Nepal
[*] Corresponding Email: narayan.adhikari@cdp.tu.edu.np

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Abstract

To study the interaction of atoms present in the two rings polymer molecule system, we have performed path integral, Monte Carlo simulations method using FORTRAN code. In literature, we found that the interaction of atoms present in two rings polymer molecule was done by path integral, Monte Carlo simulations method. Also, we found that less the number of atoms present in the rings polymer molecule i.e. P = 2, 4, 8, 16, more will be the probability of getting classical result. But, if the numbers of atoms are increased in the rings, we can reach near exact quantum mechanical result. When the value of P is ∞ the average interaction energy value of atoms present in two rings was found to be 0.5, which was exact zero point energy value of harmonic oscillator. As given in literature, we have studied the interaction of atoms present in two rings polymer system using path integral, Monte Carlo simulations method, the result we produced was as same as in literature, where the value of P were 2, 4, 8, 16 and ∞. We have done additional work by taking the values of P = 32, 64, 128, 256 and calculated the variation of average interaction energy with temperature, and found that the value of average interaction energy <E> = 0.5 at low temperature T ≈ 0K. This value is called zero point energy value of quantum harmonic oscillator. Here, the value of P = 256 and P = ∞ can resemble with each other. For this, we took P = 256 and observed the interaction, and found that the average interaction energy value of atoms present in rings was 0.5 at T ≈ 0K. Therefore, by this additional work we can say more clearly that increasing the number of atoms in two rings polymer molecule will result to the high possibility of getting exact value of average interaction energy in the system.

Keywords: FORTRAN, Path integral, Monte Carlo, Harmonic Oscillator, Interaction.

1. INTRODUCTION

Schrodinger's equation and Heisenberg's matrix mechanics are based on Hamiltonian classical mechanics, which provides a direct connection between classical and quantum mechanics [1-3]. In 1933, Dirac [4, 5] proposed an approach to quantum mechanics based on the Lagrangian, he considered it as more basic than the Hamiltonian. Dirac suggested that in quantum mechanics, transition amplitude is also known as the propagator which correlates to the quantity $e^{iS/\hbar}$ where S is the classical action calculated along the path taken by particles. In 1948, Feynman [6] extended Dirac's idea and formulated quantum mechanics based on sum over all paths between fixed initial and final states. The amplitudes of paths combined by superposition principle, in which each path contributes a pure phase $e^{iS/\hbar}$ to the propagator, as suggested by Dirac. This sum over paths is typically an integral over continuum of paths is known as path-integral method. Feynman derived the path integral methods and applied into many areas of Physics [1], most notably in non-relativistic quantum mechanics, many body Physics, quantum field theory and statistical mechanics etc. [7, 8]. In quantum mechanics, path integral leads to phenomena like tunneling, double-slit experiment etc. To interpret these experiments, path integral provides a fascinating basis [9]. Path integral is an explicit expression for the probability amplitude. The actual calculation of these amplitudes depends on the problem of interest such as harmonic oscillator, the path integral can be evaluated exactly, but typically either an approximate solution is found or a perturbative expansion is done. The various others established methods like mean field theory, renormalization group etc. are obtaining exact or approximate solution from path integrals [10], however there are some situations approximate solution are ineffective for example in Quantum Chromo Dynamics (QCD), where calculations based on perturbation theory have been successful. In the strong interaction regime provides non-perturbative numerical evaluation of amplitudes and matrix elements, which are based on Monte Carlo methods [11-13].

The Monte Carlo simulations method is a large class of algorithms that simulates quantum systems with the idea of solving the quantum many body problems like Schrodinger wave equation [14]. It makes use of random numbers to make a series of random moves, an algorithm is then used to accept or reject the move. Depending on the Monte Carlo method used, a specific function is applied to old and new configurations. The move is either accepted or rejected by comparing the results of this function before and after the move. Also, Monte Carlo simulations [15], is a method for analyzing the behavior of any activity or process that involves uncertainty so that this method is used random numbers and probability statistics to solve the problems. As we know, it may be easy to solve the equations which described the interaction between the two atoms but solving the same equations for hundreds or thousands of atoms is often impossible. Monte Carlo methods can be sampled a large system with a number of small random configurations and that data can be used to analyze the overall system.

Thus, Monte Carlo simulations method is widely used in different fields that range from economics to nuclear physics [16]. In Monte Carlo algorithms, the entire system, which may be an equation involving hundreds or thousands of variables is simulated or evaluated a large number of times. Each time the equation is simulated, the unknown variables are sampled. The system is then simulated numerous times and the performance of the system can be commutated. At the end of the simulations, the result is a large number of samples which describe the possible state of the system. These results are combined into probability distributions of possible outcomes. As a result, the outputs are not single values but probability distributions.

In this project, we focused path integral method on quantum mechanical treatment of two rings polymer system using FORTRAN code based on Monte Carlo simulations method.

2. SIMULATIONS METHOD

We have done path integral simulations of two rings polymer molecule by using Monte Carlo simulations method based on FORTRAN code. FORTRAN is a programming language which was conceived in early 1950s [17, 18]. In present work, we have considered two rings polymer molecule as a system, where P represents the number of atoms present in a system. This system is an example of Harmonic oscillator. Here, we have taken FORTRAN code for a considered polymer molecule at different values of P with different values of temperature. In this FORTRAN program, program name is given as *qmc-pi-sho.f90* which is a simple path integral, Monte Carlo simulations program. We have used this path integral, Monte Carlo simulations method to study the variation of average interaction energy between the atoms in the rings polymer molecule at different temperatures.

The *Math-module* and *average-module* in FORTRAN program are incorporated in intrinsic and others different conditions are used as a code in designed FORTRAN program. We have taken different values of P and temperature at constant values of *nstep*, *nblock*, *nequil* and *dx-max*, and also we have taken 20 numbers of blocks for production, 10 numbers of blocks for equilibration, 50000 numbers of steps per block in simulations and value 1.00 for maximum displacement in FORTRAN code. Here, we considered P is an integer and temperature, *dx-max*, and classical and quantum potentials are taken as real. This program is run in Linux by using *gfortran……f90,* we got different data and plots, and they are discussed in results and discussion section.

3. RESULTS AND DISCUSSION

In this section, we discussed the interaction of atoms in two rings polymer molecule by using path integral, Monte Carlo simulations method based on FORTRAN code and we compared our main findings, their interpretation with reported results.

3.1 Path-Integral Simulations

To arrive at the path integral formulation of quantum mechanics, we consider the problem of calculating the probability of a particle leaving a position like q_i and arriving at a position q_f under the action of a potential V(q) in a time T [16]. We used Dirac path integral formalism; the probability is given by $< q_f / e^{-iHT} / q_i >$. The interpretation is that we divide time axis in N times slices and then compute the probability amplitude for the particle leaving a position q_i at time t_i and reaching the position q_{i+1} at time t_{i+1}. The next step is to multiply these amplitudes to obtain the probability amplitude for the particle leaving q_i arrive at q_f in time T through a specific path. We repeat this for all possible paths and sum the amplitudes for each path to obtain the total probability amplitude $<q_f/e^{-iHT}/q_i>$. The path integral evaluate analytical solutions numerically, for this we relate the path integral with the partition function on statistical mechanics and use the metropolis algorithm to make Monte Carlo simulations. In our considered system, nuclei of the atoms are modeled by quantum mechanically which incorporated quantum effects in simulations [19]. So our attempts have been made to incorporate quantum effects in simulations within the limitation of classical simulations. To estimate quantum corrections of thermodynamics function by expanding the partition function of N atoms in powers of Planck constant in expression of partition function [19, 20],

$$Q_{NVT} = \frac{1}{a\Lambda^{3N}N!}\int dr[1-\frac{\beta\eta^2}{24m}\sum_{i=1}^{N}(\nabla_{r_i}\beta V(r))^2]e^{-\beta V(r)}....(1)$$

Where, $\Lambda = \left(\frac{h^2}{2\pi m K_B T}\right)^{\frac{1}{2}}$

The corrections to the thermodynamic properties, extra term is added in the classical Hamiltonian, [21] which is given by;

$$H^{qu} = H^{cl} + \frac{\eta^2\beta}{24m}[-\frac{\beta}{m}(\sum_i P_i.\nabla_{ri})^2 V^{cl} + 3\sum_i \nabla^2{}_{ri}V^{cl} - \beta\sum_i(\nabla_{ri}V^{cl})....(2)$$

But, correction term obtained was done by molecular dynamics (MD) simulation model which was numerically instabilities. Therefore, to treat the nuclei quantum mechanically, we have needed quantum partition function which is obtained by the path integral formulation of quantum mechanics, by taking non-normalize quantum mechanical density operator $\rho = e^{-\beta H}$ [1, 21, 22],

$$Q_{NVT}(\beta) \approx \frac{1}{NP!}\left(\frac{M}{2\pi\beta\eta^2}\right)^{\frac{3NP}{2}}\int dre^{-\beta V(r)}....(3)$$

Where, r represents the position of all the molecules. Using equation (3), some properties like thermodynamics properties, static and dynamic structure properties are estimated. We first take for one particle then generate to N particles then get [23] the partition function is;

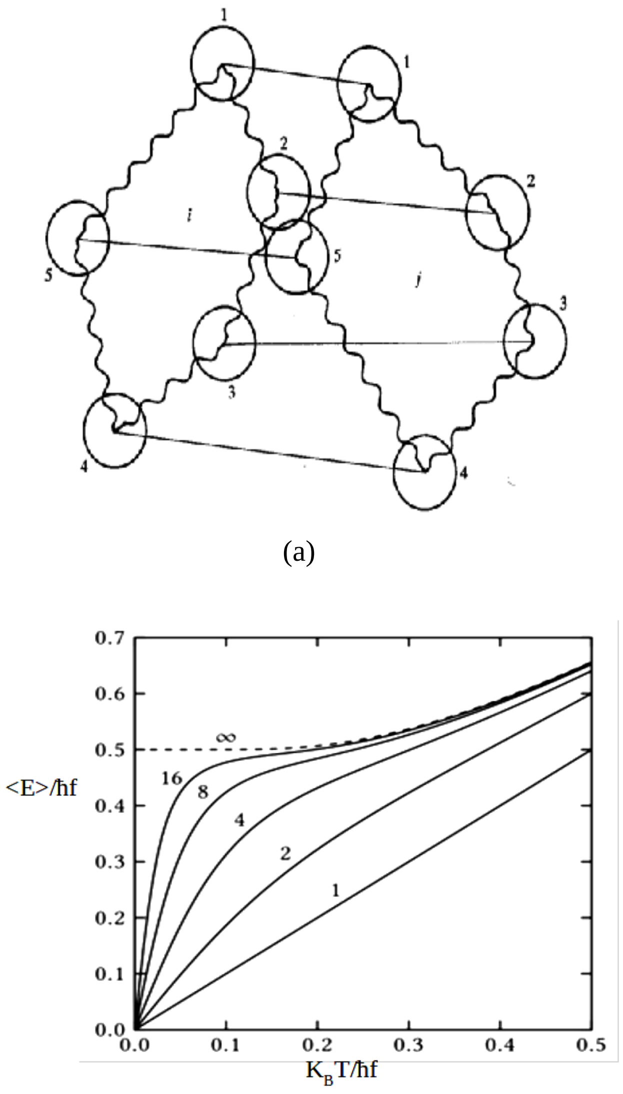
$$Q_{NVT}(\beta) \approx \frac{1}{NP!}\left(\frac{M}{2\pi\beta\eta^2}\right)^{\frac{3NP}{2}}\int dre^{-\beta V(r)}....(3)$$

Where, *mp=M*,

Or,

$$V(r) = V^{cl}(r) + V^{qu}(r)....(4).$$

Since, $V^{cl}(r)$ and $V^{qu}(r)$ represent the Classical and Quantum potential respectively. Thus, a Monte Carlo simulation of the classical ring polymer system with potential energy V(r) is given by equation (4). As the number of particles P in our ring polymer increases, we get a better approximation of quantum partition function and become formally exact as P = ∞. We can see the theoretical graph, the finite P valued energy curves deviate from the true result as temperature decreases, leaving the zero point level $E = \frac{1}{2}\eta\omega$ and dropping to classical value < E > = 0 at T = 0 as shown in Fig. 1(b) [22].



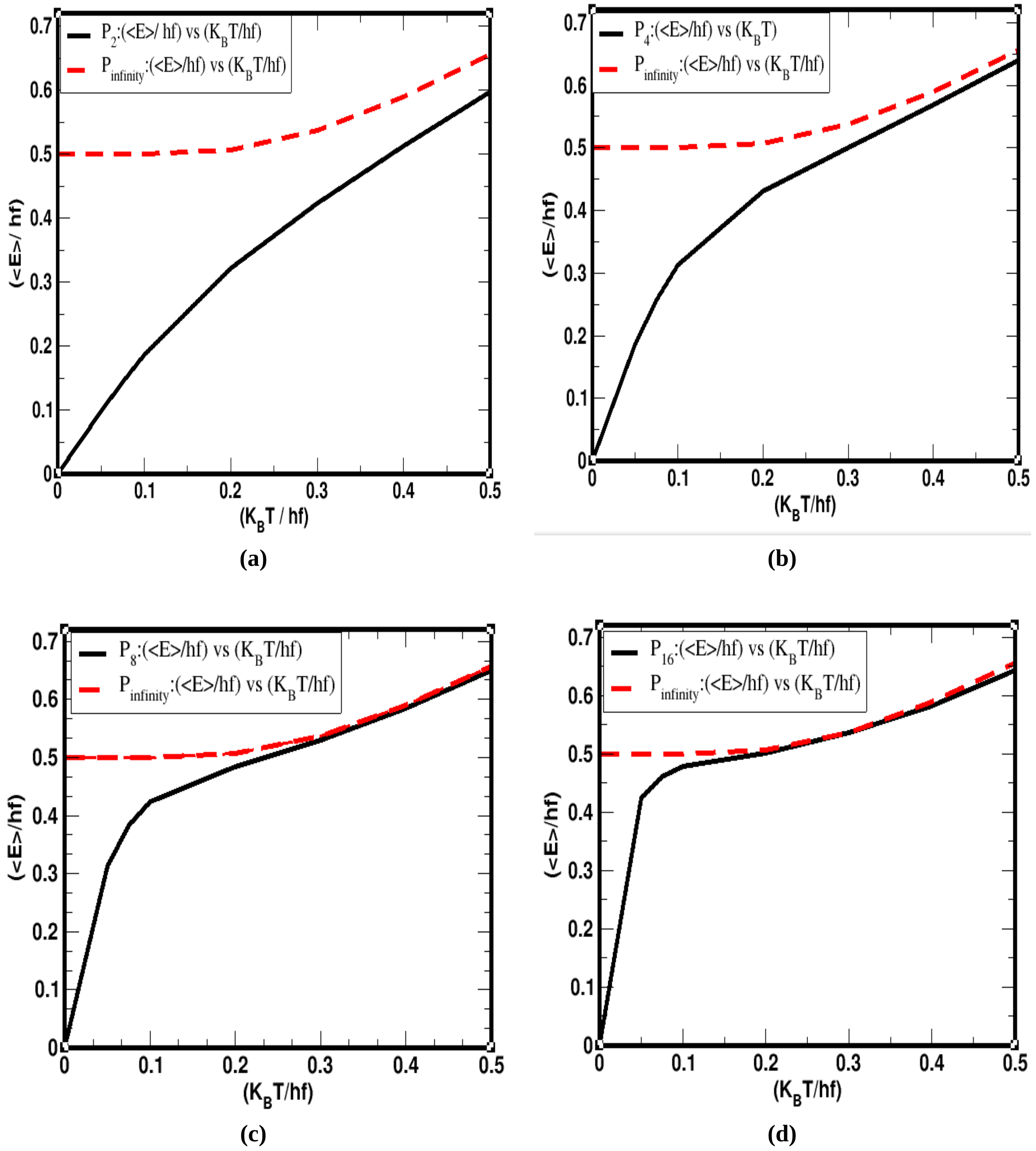
(a)

(b)

Fig. 1: *(a) Two rings polymer molecule (P = 5) representing the interaction between two atoms in a path integral simulation (b) The average energy of the path integral approximation to the Quantum Harmonic Oscillator of frequency as a function of temperature [22].*

In literature [22], we found a system of two rings polymer molecule shown in Fig. 1(a), in which atoms are presented in each ring. In Fig. 1(a), i and j represent two rings polymer structure where each ring contains P number of atoms. The atoms in one ring are interacted with atoms in another ring like a quantum harmonic oscillator since atoms having two rings are seemed to be bounded like an ideal spring. So that, the interaction between atoms present in the two rings looks like harmonic oscillator problem. The interaction of two rings polymer system was studied by path integral, Monte Carlo simulations method using FORTRAN program. The reported graph shown in Fig. 1(b) was obtained by doing path integral, Monte Carlo simulation in a considered polymer system where average interaction energy (<E>/hf) between the atoms in rings were taken along y-axis and different values of temperature (thermal energy K_BT/hf) were taken along x-axis. We saw that, number of atoms present in each ring (P = 1) in our considered system gives classical result, i.e. the value of average interaction energy was zero at zero temperature. But, we know that, quantum harmonic oscillator has zero point energy value ($\hbar\omega/2$) at zero temperature. Similarly, the value of P gradually increased up to 16, (i.e. P = 2, 4, 8, 16) also provided classical result (i.e. <E> = 0) at zero temperature, but quantum mechanically, average values of interaction energy between the atoms in two rings polymer molecule have greater value (i.e. 0.5) at low temperature region (i.e. T = 0K). It means, the value of average interaction energy between more numbers of atoms present in rings polymer using path integral, Monte Carlo simulations method provides approximate quantum mechanical result at absolute zero temperature. So that, at $P = \infty$ has given zero point energy value (<E> = 0.5) at T = 0K, shown in Fig. 1(b), otherwise (P = 2, 4, 8, 16) have slightly deviated result from quantum mechanical treatment of harmonic oscillator problem. Therefore, according to the result reported in literature, we can reach to the conclusion that, if number of atoms in two rings polymer system has greater amount, (i.e. P > >16 to ∞), the average value of interaction energy between the atoms in the rings polymer system would be 0.5 at zero temperature, which is called exact average interaction energy (zero point energy of harmonic oscillator) in the two rings polymer system.

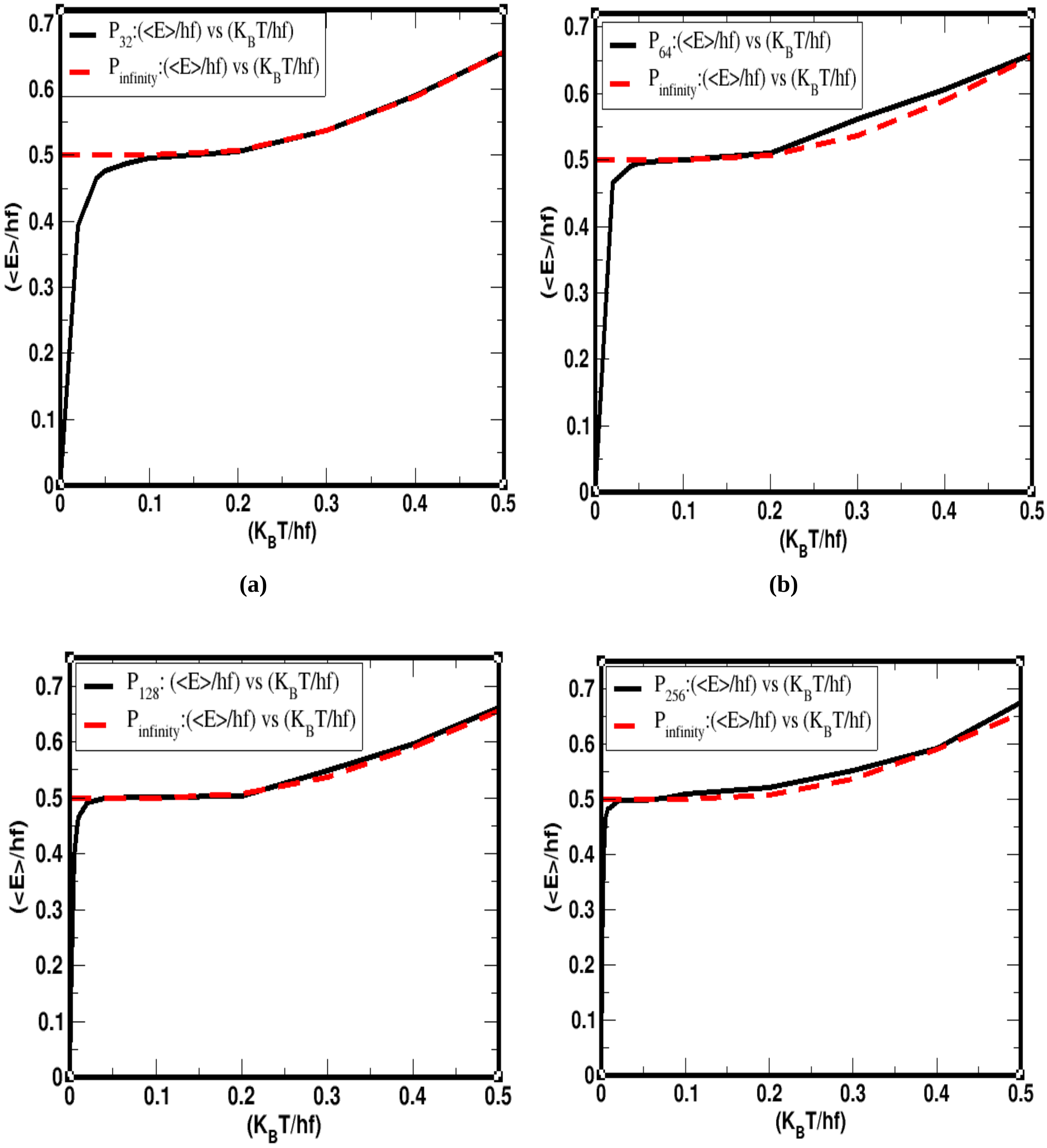
In this work, as reported in literature we have taken two rings polymer system. The atoms present in the rings interact with each other which resembles with the harmonic oscillator interaction. So that the two rings polymer system is also called an example of harmonic oscillator. Here, we have taken the number of atoms P = 2, 4, 8, 16, 32, 64, 128, 256, ∞ in our assumed system. We used path integral, Monte Carlo simulations method based on FORTRAN code to study the variation of average interaction energy of atoms in our considered system at different values of temperature. We found that, if the value of P is less (i.e. P = 2, 4, 8, 16) classical result will be obtained at T ≈ 0K as shown in Figs. 2 (a), 2(b), 2(c), 2(d) respectively. These plots are resembled exactly to the plots reported in Fig. 1(b). And, if the values of P is gradually increased from P = 32, 64, 128, 256, ……., the average interaction energy will be seen near the exact value (0.5) at T ≈ 0K temperature as shown in Figs. 3(a), 3(b), 3(c), 3(d) respectively.



(a) **(b)**

(c) **(d)**

Fig. 2*: Two rings polymer molecule represents the interaction between the atoms as an example of harmonic oscillator (a) The plot of average interaction energy at P = 2 and ∞ as a function of temperature (b) The plot of average interaction energy at P = 4 and ∞ as a function of temperature (c) The plot of average interaction energy at P = 8 and ∞ as a function of temperature (d) The plot of average interaction energy at P = 16 and ∞ as a function of temperature.*



(a) **(b)**

(c) **(d)**

Fig. 3*: Two rings polymer molecule represents the interaction between the atoms as an example of harmonic oscillator (a) plot of average interaction energy at P = 32 and ∞ as a function of temperature (b) plot of average interaction energy at P = 64 and ∞ as a function of temperature (c) plot of average interaction energy at P = 128 and ∞ as a function of temperature (d) plot of average interaction energy at P = 256 and ∞ as a function of temperature.*

Here, we have presented the simulated data of average interaction energy values of atoms in two rings polymer system at P = 2, 4, 8, 16, 32, 64, 128, 256 and ∞ with different values of temperature in table 1, where P = ∞ is obtained from the large numbers of iteration in Monte Carlo simulations method.

Table 1: Data of thermal energy in term of temperature (K_BT/hf) and average interaction energy between the atoms in i and j rings polymer molecules in term of ($<E>/hf$) are obtained from the path integral, Monte Carlo simulations method by using FORTRAN f90 program where P represents number of atoms are presented in a ring.

Temperature (Thermal energy)	Average energy (P=2)	Average energy (P=4)	Average energy (P=8)	Average energy (P=16)	Average energy (P=32)	Average energy (P=64)	Average energy (P=128)	Average energy (P=256)	Average energy (P =∞)
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.5000
0.0010	0.0002	0.0009	0.0010	0.0017	0.0089	0.0120	0.1240	0.2278	0.5000
0.0025	0.0009	0.0049	0.0079	0.0098	0.0298	0.0519	0.2695	0.3941	0.5000
0.0050	0.0028	0.0094	0.0099	0.0168	0.0860	0.1532	0.3939	0.4659	0.5000
0.0075	0.0056	0.0198	0.0343	0.0957	0.1568	0.2544	0.4435	0.4834	0.5000
0.0100	0.0099	0.0410	0.0883	0.1998	0.2056	0.3003	0.4661	0.4842	0.5000
0.0200	0.0398	0.0791	0.1524	0.2695	0.3940	0.4656	0.4910	0.4978	0.5000
0.0400	0.0788	0.1523	0.2695	0.3942	0.4661	0.4853	0.4984	0.4979	0.5000
0.0500	0.0910	0.1856	0.3124	0.4238	0.4774	0.4959	0.4988	0.4983	0.5000
0.0750	0.1436	0.2575	0.3842	0.4609	0.4887	0.4983	0.5014	0.5016	0.5000
0.1000	0.1860	0.3126	0.4241	0.4780	0.4957	0.4995	0.5020	0.5097	0.5000
0.2000	0.3220	0.4314	0.4843	0.5022	0.5061	0.5105	0.5030	0.5217	0.5078
0.3000	0.4228	0.5008	0.5292	0.5368	0.5373	0.5619	0.5482	0.5512	0.5370
0.4000	0.5123	0.5679	0.5851	0.5815	0.5902	0.6067	0.5858	0.6022	0.5894
0.5000	0.5975	0.6394	0.6501	0.6434	0.6562	0.6690	0.6643	0.6656	0.6565

According to the data we produced, variation of average interactions energy with temperature at P = 2, 4, 8, 16, 32, 64, 128, 256 and ∞ are shown in Fig. 4.

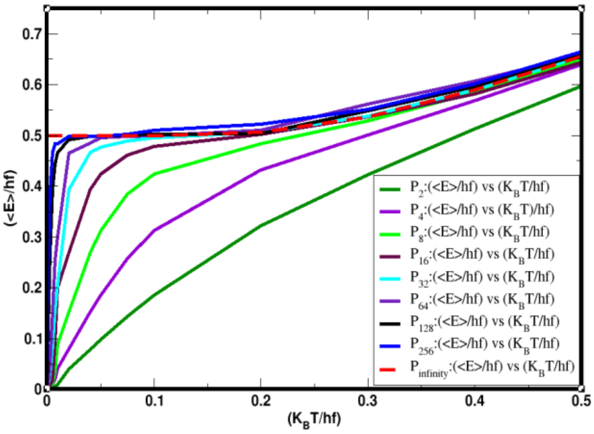


Fig. 4: *Variation of average interaction energy of atoms present in two rings polymer molecule at P = 2, 4, 8, 16, 64, 128, 256 and ∞ as a function of temperature, where values of average interaction energy are plotted along y-axis and thermal energy as a function of temperature are plotted along x-axis.*

In Fig. 4, we can see average interaction energy values of atoms in rings polymer at P = 32 is greater than 16, P = 64 is greater than 32, P = 128 is greater than 64 and P = 256 is greater than 128 at T ≈ 0K temperature. From these observations, we can be more clear that, study of the interaction between more numbers of atoms present in the two rings polymer system, will implies to reach near to exact result reported by quantum mechanics. Here, we have calculated the interaction of each atom in ring ‘i’ with all atoms in ring ‘j’ by using Monte Carlo method of simulations. As a result, there will be more chance to get accurate value of average interaction energy from large numbers of data. Hence, value of average interaction energy of atoms in rings at P = 256 is close to 0.5 than other values of P at T ≈ 0K, i.e. the value of P = 256 and P = ∞ can resemble with each other. When the interaction was observed at P = 256, we found that the average interaction energy value of atoms present in rings was 0.5 at T ≈ 0K also shown in Fig. 3(d). Therefore, by using path integral Monte Carlo simulations method based on FORTRAN code, we can reach to the conclusion that more the number of atoms present in the two rings polymer system, there will be more probability to get exact value of interaction energy (0.5) of harmonic oscillator at T = 0K.

4. CONCLUSIONS

In summary, we have studied the interaction of atoms present in two rings polymer molecule by path integral, Monte Carlo simulations method based on FORTRAN code.

We have taken two rings polymer molecule as a system for simulations, in which each ring contains P = 2, 4, 8, 16, 32, 64, 128, 256 and ∞ atoms separately. Firstly, we have taken P = 2, 4, 8, 16 atoms for simulations, and we found that, average interaction energy values of atoms in rings are decreased and reached to zero at T ≈ 0K temperature. It means, if the value of P is less (i.e. P = 2, 4, 8, 16), classical result was obtained at T ≈ 0K temperature. Additionally, we have done the simulations of P = 32, 64, 128 and 256 by using same method mentioned above and found that greater number of atoms present in the system have given nearly exact value i.e. <E> = 0.5 at T ≈ 0K, which was exact zero point energy value of harmonic oscillator problem. That exact energy of harmonic oscillator can be obtained by substituting the value of P ≈ ∞ in the system. However, in this work, the value of P = 256 is exact value near ∞. By taking this value i.e. P = 256 and observing the interaction, we found that the average interaction energy value of atoms present in rings was 0.5 at T ≈ 0K. Therefore, we can be clearer that, more the number of atoms present in the two rings polymer molecule system, the average interaction energy value of atoms in system has exact 0.5 at zero temperature. This value is called zero point energy value of quantum harmonic oscillator.

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