The rubber band revisited:  
Wang–Landau simulation

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Abstract. In this work we apply Wang–Landau simulations to a simple model which has exact solutions both in the microcanonical and canonical formalisms. The simulations were carried out by using an updated version of the Wang–Landau sampling. We consider a homopolymer chain consisting of N monomers units which may assume any configuration on the two-dimensional lattice. By imposing constraints to the moves of the polymers we obtain three different models. Our results show that updating the density of states only after every N monomer moves leads to a better precision. We obtain the specific heat and the end-to-end distance per monomer and test the precision of our simulations by comparing the location of the maximum of the specific heat with the exact results and conventional Wang–Landau simulations for the three types of walk.

Keywords: rigorous results in statistical mechanics

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1. Introduction

The sequencing of the human reference genome, announced ten years ago, provided a roadmap that is the basic foundation for modern biomedical research [1]. This monumental achievement was enabled by developments in DNA (homopolymer) sequencing technology that allowed data production which exceeds the original description of Sanger sequencing [2]. Linear polymers are the simplest physical systems that can be studied in the framework of random walk models. They are long chain-like molecules formed by repetition of a basic unit or segment, where more importantly the polymer is flexible, i.e., it can assume different geometric configurations.

Recently, the study of homopolymers has been established by various techniques in condensed matter physics. Cohen et al [3], studied the behavior of single file translocation of a homopolymer through an active channel under the presence of a driving force by using Langevin dynamics simulation. Previous works on homopolymers which studied the denaturation of circular DNA are extensions of the Poland–Scheraga model [4]. Experimentally, the viscoelastic properties of a binary mixture of a mesogenic side-chain block copolymer in a low molecular weight nematic liquid crystal are studied for mass concentrations ranging from the diluted regime up to a liquid crystalline gel state [5].

Although Monte Carlo simulations play an important role for the study of phase transitions and critical phenomena, some well-known difficulties arise when one uses standard algorithms (one-flip algorithms) [6] for the study of random walk models. These difficulties have been overcome by the development of alternative Monte Carlo methods, such as parallel-tempering [7], cluster algorithms [8], multicanonical algorithms [9], and more recently the Wang–Landau method [10]. This method has been applied with great success to many systems, in particular to polymers in a lattice [11]–[13].

In the present paper, using an updated version of the Wang–Landau method [14], we investigate the computer simulations of a homopolymer model with exact solution in a
The rubber band revisited

Figure 1. Here we consider three types of walks. (a) Model 1: unrestricted motion along the $x$-axis and $y$-axis, where the number of steps in this configuration is $N_{x}^{+} = 9$, $N_{x}^{-} = 2$, $N_{y}^{+} = 5$, and $N_{y}^{-} = 3$, (b) model 2: the backward motion on the $x$-axis is forbidden and the number of steps is $N_{x}^{+} = 7$, $N_{y}^{+} = 4$ and $N_{y}^{-} = 3$, and (c) model 3: the random walk moves only along the positive directions of $x$-axis and $y$-axis, with $N_{x}^{+} = 7$ and $N_{y}^{+} = 3$.

canonical and microcanonical formalism. One of the improvements proposed in this new way of implementing the method is that the density of states and the histogram are not updated after every trial move, but only after a Monte Carlo sweep is performed. The connection between this procedure and a better accuracy was pointed out before by Zhou and Bhatt [15].

The paper is organized as follows: in section 2 we give an introduction to the three studied models and we briefly present the mathematical background. In section 3 we outline shortly how the simulations were carried out. In section 4 we show and discuss the results for all the models and in section 5 we present our conclusions.

2. Models and formalism

2.1. Model 1

We consider a homopolymer chain of $N$ monomer units of length $a$ which may assume any configuration on a two-dimensional lattice [16]. One end of the polymer is fixed and it is taken as the origin of coordinates, shown by an open circle in figure 1(a). The other end of this linear chain is subject to an externally applied tension $\tau$, acting along the positive
$x$-axis. A possible realization of this model is sketched in figure 1(a). Each polymer unit is permitted to lie either parallel or antiparallel to the $x$-axis, and we assign the works $-\tau a$ and $+\tau a$ to these two orientations. We denote by $L_x$ the distance between the ends of the polymer chain, in the $x$-direction. Each monomer unit has the additional possibility of lying perpendicular to the $x$-axis, in the $+y$ or $-y$ directions. We associate a positive energy $\varepsilon$ to such a perpendicular monomer and the distance between the ends of the chain on the $y$-direction is denoted by $L_y$.

The Hamiltonian of this model can be written as

$$H_1 = (N^+_y + N^-_y) \varepsilon + (N^-_x - N^+_x) \tau a,$$

where $N^+_x$ and $N^-_x$ are the number of monomers along the $+x$ and $-x$ directions respectively, and similarly for $N^+_y$ and $N^-_y$. Since the tension in the $y$ direction is zero, we can assume $N^+_y = N^-_y$. Then

$$N = N^+_x + N^-_x + N^+_y + N^-_y,$$  \hspace{1cm} (2)

$$N^+_x - N^-_x = L_x,$$  \hspace{1cm} (3)

$$N^+_y + N^-_y = U,$$  \hspace{1cm} (4)

from which we find

$$N^+_x = \frac{1}{2} (N - U + L_x),$$  \hspace{1cm} (5)

$$N^-_x = \frac{1}{2} (N - U - L_x),$$  \hspace{1cm} (6)

and

$$N^+_y = N^-_y = \frac{1}{2} U.$$  \hspace{1cm} (7)

The number of configurations of the polymer consistent with a given end-to-end distance in the $x$-direction, $L_x$ (the dimensionless length of the polymer), and $U$ (the number of monomers lying perpendicular to the $x$-axis), is

$$\Omega (L_x, U, N) = \frac{N!}{N^+_x!N^-_x!N^+_y!N^-_y!}. $$

(8)

From equation (1), if we set $\varepsilon \equiv \tau a = 1$, we can write for a given energy level

$$E = U - N^+_x + N^-_x,$$  \hspace{1cm} (9)

and from equation (2)

$$N = U + N^+_x + N^-_x.$$  \hspace{1cm} (10)

Adding the equations (9) and (10) we obtain

$$U + N^-_x = \frac{N + E}{2}.$$  \hspace{1cm} (11)

Inserting equations (5), (6) and (7) into (8), using equations (9), (10), and (11), and setting $N^-_x \equiv n$ we obtain the number of configurations with energy $E$ as

$$g(E) = \sum_{u=0}^{(N+E)/2} \sum_{n=0}^{u} \frac{N!}{((N - E)/2)!((N + E)/2 - u)!n!(u - n)!},$$

\hspace{1cm} (12)

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Using the definition of the entropy and defining $\frac{\partial S}{\partial U} = \frac{1}{T}$, we obtain [16]:

$$\frac{L_x}{N} = \frac{\sinh(\tau a/k_B T)}{\cosh(\tau a/k_B T) + \exp(-\varepsilon/k_B T)}.$$ (13)

2.2. Model 2

In this model we consider that each polymer unit is parallel to the $x$-axis; no antiparallel move is allowed. Additionally the polymer units have the possibility of lying on the $+y$ and $-y$ directions. In figure 1(b) is sketched a possible configuration of this model, where we depicted by an impenetrable wall the forbidden region along the $x$-axis.

The Hamiltonian for the model 2 can be written as

$$H_2 = (N_x^+ + N_y^-) \varepsilon - N_x^+ \tau a,$$ (14)

where $N_x^+$ is the number of monomers along the $+x$ direction and similarly for $N_y^+$ and $N_y^-$. Assuming again $N_y^+ \equiv N_y^-$, we obtain the following equations:

$$N_x^+ = \frac{1}{2} (N - U + L_x)$$ (15)

and

$$N_y^+ = N_y^- = \frac{U}{2}.$$ (16)

For this model the number of configurations of the polymer consistent with a given $L_x$ and $U$ is

$$\Omega (L_x, U, N) = \frac{N!}{N_x^+!N_y^+!N_y^-!}.$$ (17)

From equation (14), if we set $\varepsilon \equiv \tau a = 1$, we can write the energy as

$$E = U - N_x^+,$$ (18)

and for $N = N_y^+ + N_y^- + N_x^+$ we obtain

$$N = U + N_x^+.$$ (19)

After similar calculations as for model 1, section 2.1, we obtain the density of states and end-to-end distance per monomer, respectively

$$g(E) = \sum_{n=0}^{(N+E)/2} \frac{N!}{((N - E)/2)!(n + (N + E)!/2)!n!}$$ (20)

and

$$\frac{L_x}{N} = \frac{1}{1 + 2 \exp(-2\tau a/k_B T)}.$$ (21)

2.3. Model 3

In this model we consider that each polymer unit is parallel to the $x$-axis and we allow only the possibility of lying on the $+y$ direction. Thus, we restrict to the situation of positive values for both axes. In figure 1(c) we show a possible configuration of this model.
The Hamiltonian for the model can be written as
\[ H_3 = N_x^+ \varepsilon - N_x^+ \tau a, \]  
where \( N_x^+ \) is the number of monomers along the \(+x\) direction and similarly for \( N_y^+ \). Again, using the method previously described, we obtain \( N_x^+ \) and \( N_y^+ \) for this model
\[ N_x^+ = \frac{1}{2} (N - U + L_x) \]  
and
\[ N_y^+ = \frac{1}{2} (N + U - L_x). \]  
For this model the number of configurations with energy \( E \) is given by
\[ g(E) = \frac{N!}{((N - E)/2)!((N + E)/2)!}. \]  
Using the equation for \( g(E) \) we obtain the length of the polymer as
\[ \frac{L_x}{N} = \frac{1}{1 + \exp(-2\tau a/k_B T)}. \]  

3. Simulations

In our simulations we followed the prescriptions of \[14\]: (a) instead of updating the density of states after every trial move, we update it after each Monte Carlo sweep; (b) Wang–Landau simulations are carried out only up to a \( \ln f = \ln f_{\text{final}} \) defined by the canonical averages during the simulations and (c) the microcanonical averages should not be accumulated before \( \ln f \leq \ln f_{\text{micro}} \) defined by the microcanonical averages during the simulation. A trial move is defined as giving sequentially to each unit the possibility of changing its state with identical probability to any allowed direction or remaining in the same one. We define a Monte Carlo sweep (MCS) as a sequence of \( N \) trial moves. As a result, a given configuration of Model 1 is a set of \( N \) monomers, each at one of the possible four states: \(+x\), \(-x\), \(+y\) or \(-y\). For Model 2 the possible states are \(+x\), \(+y\) and \(-y\) and for Model 3, only \(+x\) or \(+y\). Since the polymer is not self-avoiding, a configuration as \(+x−x+x−x\cdots+x−x\), for example is possible for Model 1 attaining \( E = 0 \). The definition of \( f_{\text{final}} \) and \( f_{\text{micro}} \) were obtained by Ferreira and Caparica \[17\], yielding \( f_{\text{final}} = f_{14} \) and \( f_{\text{micro}} = f_0 \) (the microcanonical averages may be accumulated from the very beginning). The model studied there is the same as the present Model 1, and similar tests for Models 2 and 3 lead to the same results. At the beginning of the simulation we set \( S(E) = 0 \) for all energy levels, where \( S(E) \equiv \ln g(E) \). The random walk in the energy space runs through all energy levels from \( E_{\text{min}} \) to \( E_{\text{max}} \) with a probability
\[ p(E \rightarrow E') = \min \{ \exp [(S(E) - S(E'))] \}, \]  
where \( E \) and \( E' \) are the energies of the current and the new possible configurations. After \( N \) trial moves we update \( H(E) \rightarrow H(E) + 1 \) and \( S(E) \rightarrow S(E) + F_i \), where \( F_i = \ln f_i, f_0 = e = 2.71828 \cdots \) and \( f_{i+1} = \sqrt{f_i} \) (where \( f_i \) is the so-called modification factor and \( H(E) \) is a histogram accumulated for each \( f_i \)). The flatness of the histogram is checked after a number of Monte Carlo (MC) steps, and usually the histogram is considered flat if \( H(E) > 0.8\langle H \rangle \), for all energies, where \( \langle H \rangle \) is an average over the energies. If
the flatness condition is fulfilled we update the modification factor to a finer one and reset the histogram \( H(E) = 0 \). The simulations are continued up to \( f_{\text{final}} = f_{14} \) and the microcanonical averages were accumulated from the very beginning (\( f_{\text{micro}} = f_0 \)). Having in hand the density of states, one can calculate the canonical average of any thermodynamic variable as

\[
\langle X \rangle_T = \frac{\sum_E \langle X \rangle_E g(E) e^{-\beta E}}{\sum_E g(E) e^{-\beta E}},
\]

where \( \langle X \rangle_E \) is the microcanonical average accumulated during the simulations and \( \beta = 1/k_B T \), \( k_B \) is the Boltzmann constant and \( T \) is the temperature.

4. Results and discussion

In figure 1 we depict the three models which were presented in section 2. The difference between the models is given by the allowed moves. In the first model, denoted by (a) in the figure, we allow the polymer unit to move along the positive or the negative directions of the \( x \)-axis, the same for the \( y \)-axis. The end-to-end distance of the polymer in the \( x \)-direction is denoted by \( L_x \), and with \( L_y \) we denote this distance in the \( y \)-direction. In the second model, (b) in figure 1, antiparallel motion along the \( x \)-axis is forbidden. In the third considered model there are allowed moves only on the positive side of both the \( x \)- and \( y \)-axis.

Using the simulated and the exact density of states in equation (28) we calculate the specific heat given by

\[
C = \frac{\langle (E - \langle E \rangle)^2 \rangle}{T^2}
\]

and the mean end-to-end distance

\[
\langle L_x \rangle = \langle |x_N - x_1| \rangle,
\]

where \( E \) is the energy of the configurations and \( x_1 \) and \( x_N \) are the corresponding \( x \)-coordinates of the ends of the polymer.

In figure 2 we plot on a semi-logarithmic scale the density of states \( g(E) \) for all the three models. Here we plot the results obtained from the simulations (symbols in the figure) and also the exact theoretical results (continuous lines in the figure) for a polymer of \( N = 500 \) monomers. In figure 3 we plot the end-to-end distance along the \( x \)-axis, \( L_x \), as a function of the temperature. Here we rescale \( L_x \) by the total number of monomers, \( N = 500 \) in this case. We observed a very good agreement between the simulation results (symbols in the figure) and the theoretical results (continuous lines in the figure), given by equations (13), (21), and (26), corresponding to Model 1, Model 2, and Model 3 respectively. In figure 4 we plot the specific heat per monomer for polymers with \( N = 500 \). The specific heat has a tail proportional to \( 1/T^2 \) in the high-temperature limit.

Finally, in table 1 we present the location of the peak of the specific heat for each model obtained by conventional Wang–Landau simulations (the density of states and the histogram are updated at every trial move and the simulations are continued up to \( \ln f \sim 10^{-8} \)) and the procedure adopted here and compare with the results calculated with the exact density of states. The simulations were carried out for 100 independent runs of a
polymer with $N = 100$, adopting the 80% flatness criterion. These models do not display finite size effects and the temperature of the peak of the specific heat is the same for any polymer size. Surprisingly the results obtained for $N = 100$ were more precise than for $N = 500$. One can see that in the three cases for the new procedure the exact results fall into the error bars.
Figure 4. Specific heat per monomer for polymer size $N = 500$ for (a) model 1; (b) model 2 and (c) model 3. The line is the exact result and the dots are the simulation results using the procedure for Wang–Landau simulation [17]. The error bars are smaller than the symbols.

Table 1. Temperatures of the peak of the specific heat from conventional WL simulations and the new procedure, compared with the exact values.

| Model   | Model 1 | Model 2 | Model 3 |
|---------|---------|---------|---------|
| Exact   | 0.70299027 | 0.75335362 | 0.83180562 |
| Conv. WL | 0.6990(25) | 0.7560(29) | 0.8275(28) |
| Present work | 0.7043(23) | 0.7525(25) | 0.8295(23) |

5. Conclusions

We have carried out Wang–Landau simulations of a simple polymer model which has exact solutions in both the microcanonical and the canonical ensembles. Here we considered three two-dimensional models: in the first model we allowed moves in all possible directions, in the second model moves along the negative $x$-axis are forbidden, while in the last model we allowed only moves along the positive direction for both $x$ and $y$-axis. We have shown that updating the density of states only after each $N$ trial moves and halting the simulations when $f_{\text{final}} = f_1$ [17], defined during the simulations, we obtain quite accurate results compared with the available analytical exact results. We have obtained a very good agreement between the simulations and the exact results also for the studied physical quantities: the end-to-end distance and the specific heat. As expected, due to the difference of the allowed directions of motion, in the limit of high temperatures the end-to-end distance has the highest value for the third model and the lowest for the first model.

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