

# Recursive Speed-up in Partition Function Evaluation

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## Abstract

We present a simple recursive relation that leads to the speed-up of numeric procedures for the calculating of partition functions of a generic theory. The obtained results are demonstrated for the case of the anharmonic oscillator in one dimension.

## 1 Introduction

Path integrals represent the natural framework in which to cast statistical mechanics and quantum field theory models. Unfortunately, except in the simplest cases, path integrals can not be exactly calculated using analytical methods. We are left only with numerical procedures in which partition functions are evaluated [1, 2] as a series of  $N$ -fold integrals using standard Monte Carlo methods [3]. For this reason we have been investigating various means for the speed up of such calculations. The present work represents a follow up of our previous papers [4], and focuses on path integrals in one dimension.

## 2 Formalism

We study a generic statistical model with energy of the form

$$E = \int_0^\beta d\tau \left( \frac{1}{2} G(q) \dot{q}^2 + V(q) \right) . \quad (1)$$

The corresponding partition function is calculated as a path integral over paths in imaginary time  $\tau$  going from  $q(0) = 0$  to  $q(\beta) = a$  using the standard prescription of time discretization into  $N$  equal steps of  $\epsilon = \beta/N$ . Its value  $Z$  is the large  $N$  limit of

$$Z_N = \int \prod_{n=1}^{N-1} (dq_n) \prod_{n=0}^{N-1} \left( \frac{G\left(\frac{q_{n+1}+q_n}{2}\right)}{2\pi\epsilon} \right)^{1/2} \exp(-E) , \quad (2)$$

where the discretized energy equals

$$E = \sum_{n=0}^{N-1} \left( \frac{1}{2\epsilon} G\left(\frac{q_{n+1}+q_n}{2}\right) (q_{n+1} - q_n)^2 + \epsilon V\left(\frac{q_{n+1}+q_n}{2}\right) \right) . \quad (3)$$

The expression for  $Z_{2N}$  may be cast into the same form as eq. (2) by formally integrating out all the odd indexed  $q$ 's. In this way we find

$$Z_{2n}[E] = Z_N[\bar{E}] , \quad (4)$$

where we have made explicit the dependence of partition functions on the functional form of the energy.

A relation such as the one above is obviously useful for investigating the continuum limit of the partition function – the difficulty, however, is in evaluating the effective energy  $\bar{E}$ , i.e. in explicitly doing the integrals over odd indexed  $q$ 's. It is impossible to do these intermediate integrals exactly, what we have done is to evaluate them by expanding the  $q_{2m+1}$  integrand up to quadratic terms in  $q_{2m+2} - q_{2m+1}$  and  $q_{2m+1} - q_{2m}$ . The resulting integrals are Gaussian. Doing them we obtain a closed form expression for  $\bar{E}$ . Furthermore, the effective energy  $\bar{E}$  is found to be of the same form as the starting energy  $E$ , but with modified kinetic and potential terms given by

$$\bar{G} = \mathcal{G}(G, V; \epsilon) \equiv G - \frac{\epsilon}{16} \left( \frac{G''}{G} - \left( \frac{G'}{G} \right)^2 \right) + \frac{\epsilon^2}{16} V'' , \quad (5)$$

$$\bar{V} = \mathcal{V}(G, V; \epsilon) \equiv V - \frac{1}{32\mathcal{G}} \left( \frac{G'}{G} - \epsilon V' \right)^2 + \frac{1}{2\epsilon} \ln \left( \frac{\mathcal{G}}{G} \right) . \quad (6)$$

We can now apply the above procedure recursively. To do this we start from  $N = 2^s$  imaginary time slices and obtain the following equations of descent

$$Z_N[E^{(0)}] = Z_{N/2}[E^{(1)}] = Z_{N/4}[E^{(2)}] = \dots = Z_1[E^{(s)}] , \quad (7)$$

where  $E^{(0)} = E$ , while  $E^{(1)}, E^{(2)}, \dots, E^{(s)}$  are determined through the recursive relation

$$G^{(k+1)} = \mathcal{G}(G^{(k)}, V^{(k)}; 2^{k+1}\epsilon) , \quad (8)$$

$$V^{(k+1)} = \mathcal{V}(G^{(k)}, V^{(k)}; 2^{k+1}\epsilon) . \quad (9)$$

We will not make a detailed investigation of the validity of the above approximations in this short paper. Let us only note in passing that the errors associated with using Gaussian approximations in deriving equations (5) and (6) vanish with the increase of  $N$ . Numerical evidence suggests that these errors vanish as  $O(N^{-2})$ , or even faster.

### 3 Numerical Results

In the remainder of this paper we will illustrate the usefulness of the obtained results in the case of a one dimensional anharmonic oscillator in magnetic field  $B$ . Its energy is given by

$$E = \int_0^\beta d\tau \left( \frac{1}{2} \dot{q}^2 + \frac{1}{2} q^2 + \frac{1}{4!} g q^4 - Bq \right) . \quad (10)$$

All the plots that follow are for  $B = 1$  and  $a = 1$ . All the numerical calculations were done with  $10^7$  Monte Carlo steps. Note that  $Z_{N,k}$  is simply shorthand for  $Z_N[E^{(k)}]$ . Figure 1

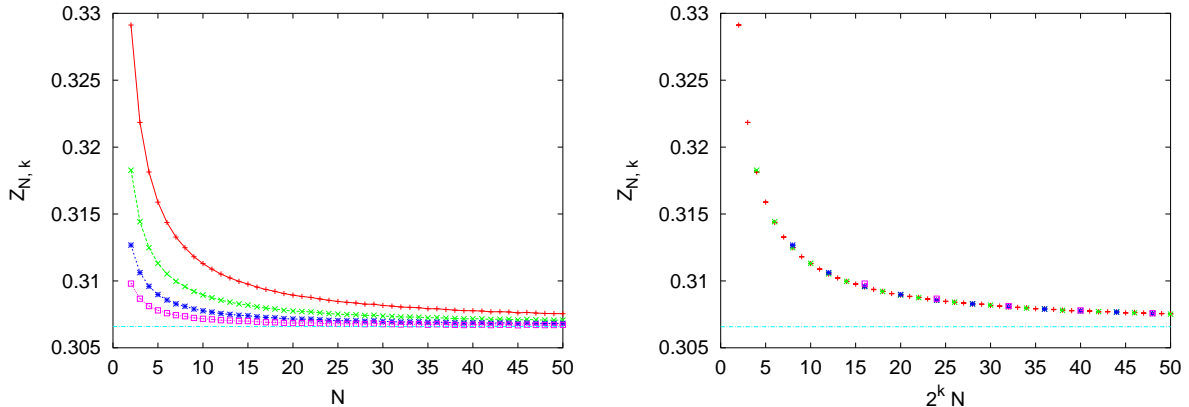


Figure 1: Plots for  $g = 1$ ,  $\beta = 1$ . Left:  $Z_{N,k}$  for  $k = 0, 1, 2, 3$ . Right: The same data collapsed to a single curve.

gives the numerical results for moderate values of coupling and temperature, i.e.  $g = 1$  and  $\beta = 1$ . The top curve on the left plot is that of  $Z_N$  as a function of  $N$ . We have obtained  $Z$  by fitting these points to the curve

$$Z_N = Z + A/N + B/N^2 + C/N^3 . \quad (11)$$

The three curves immediately below this one are of  $Z_{N,k}$  with  $k = 1, 2$  and  $3$  (from top to bottom). Each of these curves leads to the same extrapolated value of  $Z$ , shown as a horizontal line, with precision of six decimal places. Note that every consecutive curve tends to the continuum result twice as fast as the previous one. The plot on the right shows how well our Gaussian approximation is doing the job, i.e. how well eq. (7) is satisfied. It is gratifying to see that all the  $Z_{N,k}$  collapse on a single curve when plotted as functions of  $2^k N$ . Although this is to be expected for large enough  $N$ 's, we see from the above plot that this holds extremely well even for  $N = 2$ , the case of only one integral. One might assume that the approximation made in this paper is similar to the usual mean field approximation – in both cases we put the partition function into the form of a Gaussian. However, the two schemes are in fact quite different. Our derivation assumes that  $q(\tau + d\tau) - q(\tau)$  is small, while the mean field approximation assumes that  $q(\tau) - q_{mf}(\tau)$  is small. To see the difference we next look at the case of an extremely strong coupling, i.e.  $g = 100$ ,  $\beta = 1$ . The left plots of Figure 2 show that even in this strongly non-linear regime (in which the mean field result is not a good approximation) all of the given curves tend to the same continuum limit. Once again we have all the benefits of using  $E^{(k)}$  with larger values of  $k$  instead of the starting energy  $E^{(0)}$ . More importantly, the right plot shows that, as in the previous case, the deviation from the

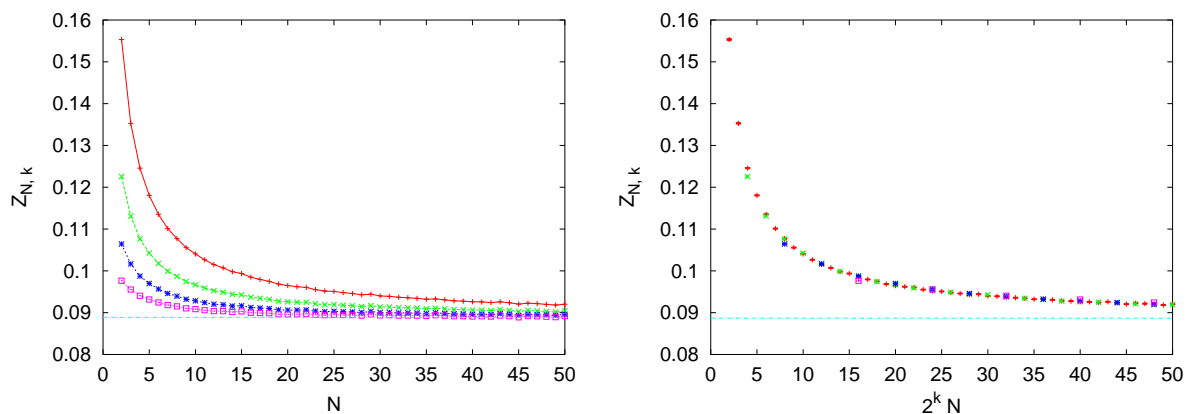


Figure 2: The case of strong coupling ( $g = 100, \beta = 1$ ).

equation of descent is extremely small even for the smallest values of  $N$ . The same is true for the case of low temperatures. Figure 3 illustrates the numerical calculations done for  $g = 1, \beta = 10$ .

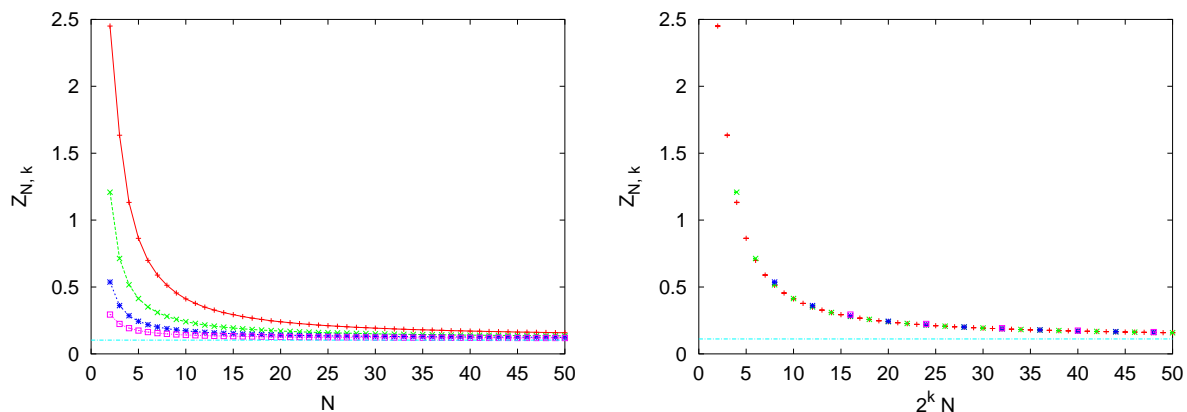


Figure 3: The case of low temperatures ( $g = 1, \beta = 10$ ).

## 4 Conclusion

In conclusion, we have obtained simple recursive relations that allow for a straightforward speed-up of the process of calculating partition functions. The uncovered results are general, i.e. they are valid for a wide class of one dimensional models, and work regardless of the strength of coupling and of temperature.

We plan to extend these results to the important case of two dimensional models. We do not foresee problems in doing this since the crucial point in the present derivation, namely the integrating out of odd indexed coordinates using the Gaussian approximation, extends naturally to higher dimensions.

## References

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