RECURSIVE SPEED-UP OF PATH INTEGRAL CALCULATIONS

A. Balaž, A. Belić and A. Bogojević
Institute of Physics, P.O.B. 57, Belgrade 11001, Yugoslavia

Abstract

We present a simple recursive relation that leads to the speed-up of numeric procedures for the calculating of path integrals of a generic quantum theory. The obtained results are demonstrated for the case of the quantum anharmonic oscillator.

Path integrals play a central role in many areas of physics, most notably in statistical mechanics and quantum field theory where they represent the natural formalism in which to cast the theory. 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 the path integral is calculated [1] as a series of N-fold integrals evaluated by standard Monte Carlo methods [2], the path integral being the continuum limit of that series.

We study a generic quantum mechanical model with Euclidean action of the form $I = \int_0^T dt \left(\frac{1}{2} G(q) \dot{q}^2 + V(q)\right)$. The corresponding path integral is calculated using the standard prescription of time discretization into N equal steps of $\epsilon = T/N$. Its value Z is the large N limit of

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

where the discretized action equals

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

The expression for $Z_{2N}[I]$ may be cast into the same form as eq. (1) by formally integrating out all the odd indexed q's. In this way we find

$$Z_{2n}[I] = Z_N[\bar{I}] . \qquad (3)$$

A relation such as the one above is obviously useful for investigating the continuum limit of path integrals – the difficulty, however, is in evaluating the effective action $\bar{I}$, 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 $\bar{I}$. Furthermore, $\bar{I}$ is found to be of the same form as the starting action I, but with modified kinetic and potential terms given by

$$\bar{G} \;=\; \mathcal{G}(G, V; \epsilon) \equiv G - \frac{\epsilon}{16}\left(\frac{G''}{G} - \left(\frac{G'}{G}\right)^2\right) + \frac{\epsilon^2}{16}\,V'' \,, \tag{4}$$

$$\bar{V} \;=\; \mathcal{V}(G, V; \epsilon) \equiv V - \frac{1}{32\mathcal{G}}\left(\frac{G'}{G} - \epsilon\,V'\right)^2 + \frac{1}{2\epsilon}\ln\left(\frac{\mathcal{G}}{G}\right) \,. \tag{5}$$

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

$$Z_N[I^{(0)}] = Z_{N/2}[I^{(1)}] = Z_{N/4}[I^{(2)}] = \ldots = Z_1[I^{(s)}] \,, \tag{6}$$

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

$$G^{(k+1)} \;=\; \mathcal{G}(G^{(k)}, V^{(k)}; 2^{k+1}\epsilon) \,, \tag{7}$$

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

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 (4) and (5) vanish with the increase of N.

In the remainder of this paper we will illustrate the usefulness of the obtained results in the case of the anharmonic oscillator with action $I = \int_0^T dt \left(\frac{1}{2}\dot{q}^2 + \frac{1}{2}q^2 + \frac{1}{4!}g\,q^4 - jq\right)$. All the plots that follow are for $j = 1$. All the numerical calculations were done with 10^7 Monte Carlo steps. Note that $Z_{N,k}$ is simply shorthand for $Z_N[I^{(k)}]$. Figure 1 gives the numerical results for $g = 1$ and $T = 1$. 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 $Z_N = Z + A/N + B/N^2 + C/N^3$. The three curves immediately bellow this
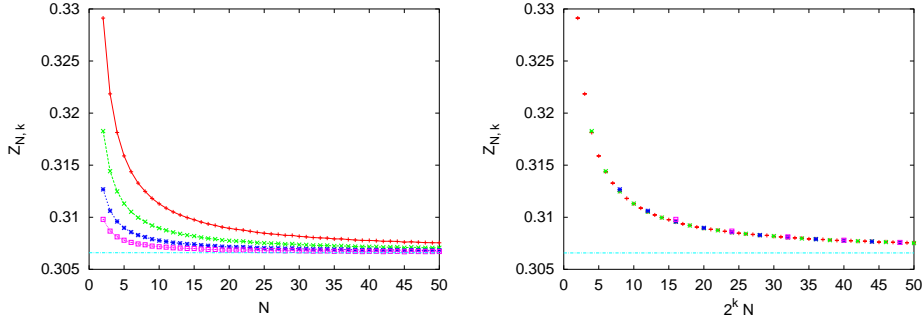
Figure 1: Plots for $g = 1$, $T = 1$. Left: $Z_{N,k}$ for $k = 0, 1, 2, 3$. Right: The same data collapsed to a single curve.

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 is eq. (6) 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
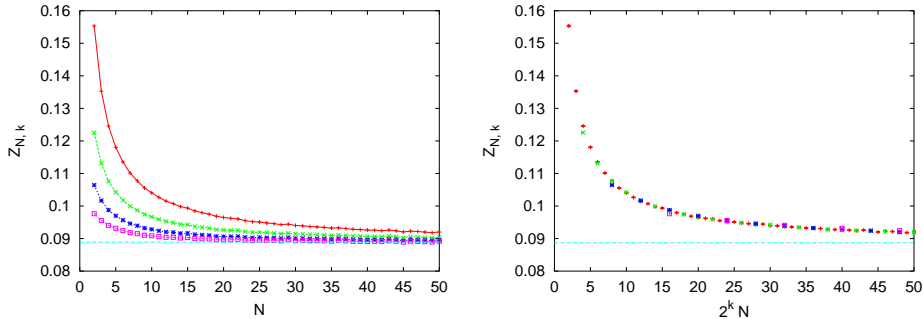

Figure 2: The case of strong coupling ($g = 100$, $T = 1$).

the usual one-loop approximation of path integrals – in both cases we put the path integral into the form of a Gaussian. However, the two schemes are in fact quite different. Our derivation assumes that $q(t + dt) - q(t)$ is

3

small, while the one-loop approximation assumes that $q(t) - q_{classical}(t)$ is small. To see the difference we next look at the case of an extremely strong coupling, i.e. $g = 100$, $T = 1$. The left plots of Figure 2 show that even in this strongly non-linear regime (in which the one-loop 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 $I^{(k)}$ with larger values of k instead of the starting action $I^{(0)}$. More importantly, the right plot shows that, as in the previous case, the deviation from the equation of descent is extremely small even for the smallest values of N. The same is true for the case of long times of propagation. Figure 3 illustrates the numerical calculations done for $g = 1$, $T = 10$. In conclusion, we have obtained
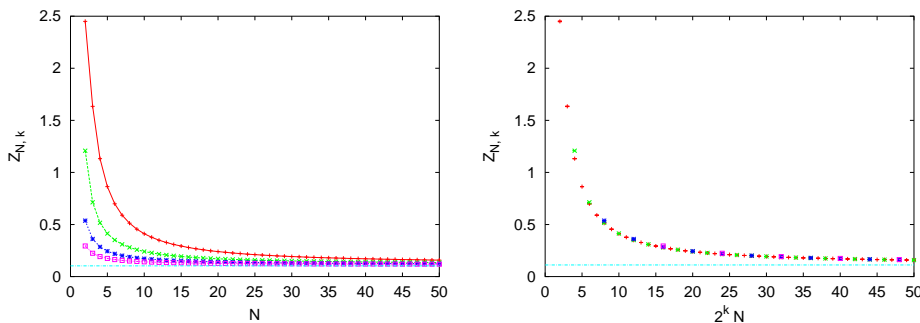

Figure 3: The case of long time propagation ($g = 1$, $T = 10$).

recursive relations that allow for a straightforward speed-up of the process of calculating path integrals. The uncovered results are general, i.e. they are valid for a wide class of models, and work regardless of the strength of coupling. The present paper, a follow up of our previous work [3], has focused on path integrals in quantum mechanics, i.e. field theory in one dimension.

References

[1] R. P. Feynman and A. R. Hibbs, *Quantum Mechanics and Path Integrals*, McGraw-Hill, New York, 1965.

[2] M. H. Kalos and P. A. Whitlock, *Monte Carlo Methods*, Vol. 1: Basics, John Wiley and Sons, New York, 1986.

[3] A. Balaž, A. Belić, A. Bogojević, SFIN A2 (1998); Phys. Low-Dim. Struct. **5/6** (1999), 1; *Ibid.* **9/10** (1999), 149; *Ibid.* **1/2** (2000), 65.