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Gaussian Halving of Path Integrals in *d*=1

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We study the error associated with the recently developed method of Gaussian halving [1] for calculating path integrals in a general theory in d=1. We show that it is of order $O(1/N^2)$ - an improvement over the standard $O(1/N)$ error of approximating the path integral of a continuum amplitude with its corresponding discretized expression in the mid-point prescription. The obtained generic results are illustrated by the case of an anharmonic oscillator.

1. Gaussian Halving

The most compact form of any quantum theory is to write it in terms of probability amplitudes written as Feynman path integrals, i.e. as the limit $Z[S] = \lim_{N\to\infty} Z_N[S_{D,N}]$, where $S_{D,N}$ is the energy functional (action) of the theory standardly discretized to N inverse temperature slices. In coordinate space we have

$$Z_N[S_{D,N}] = \int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} dq_1\cdots dq_{N-1}\,\mu[q_0,\ldots,q_N]\exp\{-S_{D,N}[q_0,\ldots,q_N]\}. \quad (1)$$

In the above expression $\mu[q_0,\ldots,q_N]$ is the measure depending on the discretized coordinates $q_0,\ldots,q_N$ and the form of the action of the theory [2, 3]. We have developed a new method, which we call Gaussian halving [1, 4] for calculating path integrals for generic theories. In this paper we present the new method for the case of statistical mechanics models in one dimension. The class of models which we investigate has Hamiltonians of the form $H = \frac{1}{2}G(q)\dot{q}^2 + V(q)$. The generic representative of this class of theories is determined through specifying the pair of functions G and V. The path integral measure for this class of theories in the mid-point prescription is

$$\mu[q_0,\ldots,q_N] = \prod_{i=0}^{N-1}\sqrt{\frac{G\left(\frac{q_{i+1}+q_i}{2}\right)}{2\pi\varepsilon_N}},$$

where $\varepsilon_N = \beta/N$.

If we take the expression for the functional integral with N slices and formally integrate out every other variable we obtain an identity linking two discretizations of the same theory - one with N and the other with $N/2$ slices. Repeating this procedure we find

$$Z_N[S_{D,N}] = Z_{N/2}[S^{(1)}_{D,N/2}] = Z_{N/4}[S^{(2)}_{D,N/4}] = \cdots.$$

If the above integrations were not formal, i.e. if we could actually do them, then the outlined halving procedure would give us explicit expressions for the effective actions $S_{N,s} = S^{(s)}_{D,N/2^s}$. In this way it would be possible to use a 2^s times courser discretization using $S_{N,s}$ and obtain the same result that we would get from the initial discretization of the starting action.

The Gaussian halving method [1, 4] approximates the outlined integrals with Gaussian integrals by expanding

the discretized action in the mid-point prescription up to quadratic terms in the differences $q_{i+1} - q_i$. In this way it becomes possible to solve all the integrals. The analytical justification for the above approximation is quite straightforward - the short time evolution of any theory gives $(q_{i+1} - q_i)^2 \propto \varepsilon_N$, where ε_N denotes a short step, which is the basic characteristic of a random walk or of a general diffusion process. Therefore, the approximation behind the Gaussian halving method becomes better with increasing values of *N*. We wish to point put that the new approximation differs from the standard semi-classical expansion (mean field approximation). Both methods approximate path integrals with Gaussian integrals but they do this through expanding the action around different points. Semi-classical expansion expands the action around the mean field, while Gaussian halving assumes that what are small are the differences of the coordinates across neighboring slices.

The second key feature of Gaussian halving is that it leads to effective actions that belong to the same class as the starting action. In this way a rather straightforward calculation leads us to a recursive relation that connects the starting action with a series of effective actions $S_{N,1}$, $S_{N,2}$, $S_{N,3}$, etc. In the case of an initial discretization with 2^s slices we get [1]

$$G_s^{(k+1)} = \mathrm{G}\left[G_s^{(k)}, V_s^{(k)}, \frac{\varepsilon_N}{2^{s-k-1}}\right], \quad (2)$$

$$V_s^{(k+1)} = \mathrm{V}\left[G_s^{(k)}, V_s^{(k)}, \frac{\varepsilon_N}{2^{s-k-1}}\right], \quad (3)$$

where

$$\mathrm{G}[G, V, \varepsilon_N] = G - \frac{\varepsilon_N}{16}\left[\frac{G''}{G} - \left(\frac{G'}{G}\right)^2\right] + \frac{\varepsilon_N^2}{16}V'', \quad (4)$$

$$\mathrm{V}[G, V, \varepsilon_N] = V + \frac{1}{\varepsilon_N}\ln\frac{\mathrm{G}}{G} - \frac{\left(\frac{G'}{G} - \varepsilon_N V'\right)^2}{32\,\mathrm{G}}. \quad (5)$$

In the above expressions $k = 0, 1, 2, \ldots, s$, and $k = 0$ corresponds to the functions *G* and *V* from our starting action.

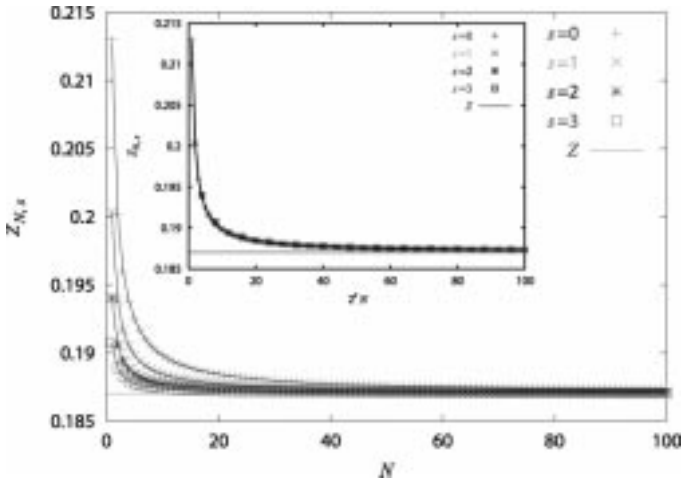

Fig. 1. Approximate values $Z_{N,s}$ ***for the partition function as functions of the number of slices N. Here the parameters of the theory are*** $g = 1$, $B = 0$, $\beta = 1$, ***while the number of Monte Carlo steps was*** $N_{MC} = 10^7$. ***The inset graph shows that the scaling relation underlying the halving procedure holds very well***

2. Numerical results

We have checked the new method by considering the example of an oscillator with quartic anharmonicity g in a wide range of parameters g, β (inverse temperature) and B (external field), as well as for a variety of boundary conditions q_0 and q_N. All results were obtained using Monte Carlo simulations [5, 6].

Fig. 1 shows how the approximate values for a discretized functional integral depends on the number of slices N. It is apparent that by increasing s (number of iterations of our recursive relation), the expressions $Z_{N,s}$ converge faster to the same continuum limit.

In the inset graph $Z_{N,s}$ is plotted as a function of $N_{eff} = 2^s N$. The fact that all the points collapse to the same curve shows us just how well the Gaussian halving procedure is working. At the same time it explains why effective actions speed up the convergence to the continuum limit - N_{eff} is what we need to increase, and we can do that

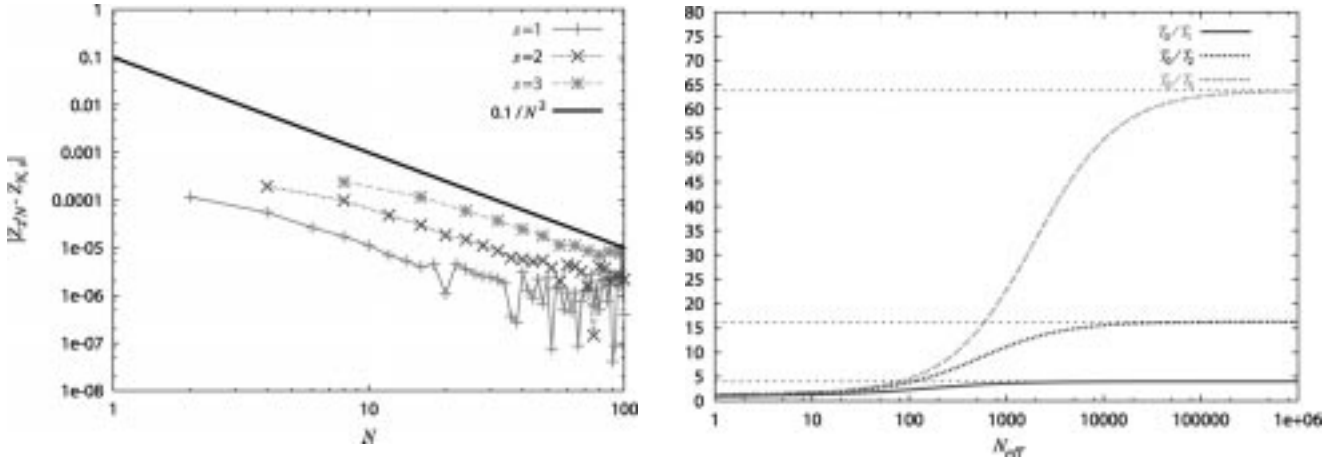

Fig. 2. (left) Absolute value of the error associated with Gaussian halving for iterates $s = 0, 1, 2, 3$.
For illustration of the 1/N² dependence of the error we have also shown the curve 0.1/N². (right) Ratio of computation times for simulations using the starting action T_0 ***and the s-th iterate,*** T_s ***i.e. the speedup. The parameters in this plot were*** $g = 1$, $B = 0$, $\beta = 1$, ***while the number of Monte Carlo steps was*** $N_{MC} = 10^7$

either by increasing N (computer time scales as N^2) or by doing a few more iterations of our recursive relation. The same behavior is found for all values of the parameters.

The error associated with the use of the Gaussian halving method can be seen from the left hand side of Fig. 2. We find that the method has an error proportional to $1/N^2$, i.e. negligible as compared to the dominant term in the $1/N$ expansion of Z_N about its continuum value $Z_N = Z + a/N + b/N^2 + O(1/N^3)$.

It is this subdominant character of the Gaussian halving error which has all the data points falling onto a single curve depending only on . On the other hand, this analytical improvement translates in the numerical approach into the faster computation of path integrals (for the same precision). This is illustrated in the right hand side of Fig. 2.

From the plot we see that by using instead of the starting action we get a significant speedup. For larger values of N the speedup becomes 4^s, which may easily be understood if we have in mind that the computing time for the Monte Carlo algorithm used is proportional to N^2.

3. Conclusion

We have presented the derivation of a general method for a more efficient calculation of path integrals. The method has been analyzed in detail for the case of quantum theories in d=1 dimensions. The analytical approximation employed in the Gaussian halving method is subdominant ($O(1/N^2)$) as compared to the expansion of Z_N about its continuum value ($O(1/N)$). This analytical procedure makes it possible to iterate the derived recurrence relations and in this way to significantly speed up path integral calculations. Although derived analytically, the recurrence relation is non-linear and in this paper we have solved it numerically. We leave the analytical treatment of the Gaussian halving recurrence relation to a following publication.

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Linearized Gaussian Halving in *d*=1

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We present an extension of a new Gaussian halving method for the calculation of path integrals introduced in Refs. [1-3]. The original method leads to recursion relations that are nonlinear and could not be solved analytically. In this paper we present a general analytical solution (including the continuum limit) of linearized recursions. We show that the error associated with this linearization is of the order $O(1/N^2)$, where N is the number of discretized steps, i.e. it is of the same order of magnitude as the error inherent in the derivation of the original method. Using this result we derive an improved algorithm for calculation of path integrals.

1. Linearized Recursion

In a series of previous papers [1-4] we have shown that in the case of quantum theories described by Hamiltonians of the form $H = \frac{1}{2} G(q)\dot{q}^2 + V(q)$ the solution of the associated path integral can be substantially sped up through iterating the recursion relation

$$G_s^{(k+1)} = \mathrm{G}\left[G_s^{(k)}, V_s^{(k)}, \frac{\varepsilon_N}{2^{s-k-1}} \right], \tag{1}$$

$$V_s^{(k+1)} = \mathrm{V}\left[G_s^{(k)}, V_s^{(k)}, \frac{\varepsilon_N}{2^{s-k-1}} \right], \tag{2}$$

where s is any positive integer, $k = 0, 1, 2, \ldots, s$, and functions G and V are given by

$$\mathrm{G}[G, V, \varepsilon_N] = G - \frac{\varepsilon_N}{16}\left[\frac{G''}{G} - \left(\frac{G'}{G} \right)^2 \right] + \frac{\varepsilon_N^2}{16} V'', \tag{3}$$