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Path Integrals and Euler Summation Formula

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Abstract

Recently introduced analytical method for systematic improvement of the convergence of path integrals of a generic N-fold discretized theory [1, 2] is presented and an Euler summation formula for path integrals is derived. The approximation made by the using of the first p terms of this formula greatly speed–up convergence of path integrals to the continuum limit: from standard $1/N$ behavior, the convergence is improved to $1/N^p$.

1 Introduction

Feynman's path integrals have, since their inception [3], represented an extremely compact and rich formalism for dealing with quantum theories. They have been powerful tools for dealing with symmetries (including gauge symmetry), for deriving non-perturbative results, for showing connections between different theories or different sectors of theories [4, 5]. Their flexibility and intuitive appeal have allowed us to generalize quantization to ever more complicated systems. As a result, path integrals have led to a rich cross fertilization of ideas between high energy and condensed matter physics [6]. Today, they are used both analytically and numerically [7, 8] in many other areas of physics, chemistry and materials science. An extensive review of path integrals and their applications can be found in [9].

The bad news is that we still have very little knowledge of the precise mathematical properties of path integrals. In addition, a very small number of path integrals can be solved exactly. The definition of path integrals as a limit of multiple integrals makes their numerical evaluation quite natural. The most all-around applicable numerical method for such calculations is based on Monte Carlo simulations.

Several research groups have in the past focused on improving the convergence of path integrals. The best available result for a generic theory (valid only for partition functions and not for general amplitudes) is the convergence of N-fold discretized expressions as $1/N^4$ [10, 11].

In order to further significantly speed up numerical procedures for calculating path integrals for a generic theory it is necessary to add new analytical input. We present and comment on the systematic investigation of the relation between different discretizations of a given theory derived in [1,2]. A result of this investigation is a procedure for constructing a series of effective actions $S^{(p)}$ having the same continuum limit as the starting action S, but which approach that limit as $1/N^p$. Using this procedure we have obtained explicit expressions for these effective actions for $p \leq 10$. In the current paper we cast the new analytical input in the form of a Euler summation formula for path integrals.

2 Ordinary Integrals

The current status of the development of the path integral formalism is quite similar to that of ordinary integrals before the setting up of integration theory by Riemann. In those days integrals were calculated directly from the defining formula, i.e. one looked at a specific discretization of the integral (Darboux sum), attempted to do the sum explicitly, and finally tried to calculate the continuum limit. For example,

$$I[f] \equiv \int_0^T f(t)dt = \lim_{N\to\infty} I_N[f]\,, \quad \text{where } I_N[f] = \sum_{n=1}^{N} f(t_n)\epsilon_N\,, \tag{1}$$

$\epsilon_N = T/N$ and $t_n = n\epsilon_N$. The last great step in the development of integration before Riemann was made by Euler. Let us briefly state Euler's summation formula that we will generalize to path integrals in the following sections.

Discretization is not unique. This makes it possible to change $f(t)$ to some other function (adding terms proportional to ϵ_N, ϵ_N^2, etc.) without changing the integral. Let us assume that $f^*(t)$ is such an equivalent function with the added property that the sums $I_N[f^*]$ do not depend on N. Then it follows that

$$\int_0^T f(t)dt = \sum_{n=1}^{N} f(t_n)\epsilon_N - \frac{\epsilon_N}{2}\sum_{n=1}^{N} f'(t_n)\epsilon_N - \frac{2\epsilon_N^2}{3}\sum_{n=1}^{N} f''(t_n)\epsilon_N + \ldots\,. \tag{2}$$

This is the well-known Euler summation formula. We may also write it more compactly as

$$I[f] = I_N[f^{(p)}] + O(\epsilon_N^p)\,, \tag{3}$$

where $f^{(p)}$ is the truncation of f^* to the first p terms. The Euler formula gives the analytical relation between integrals and their discretized sums. Looked at numerically, this formula allows us to increase the speed of convergence of discretized expressions to the continuum limit: in the defining relation the discretized expressions differ from the continuum by a term of order $O(1/N)$; by using the Euler sum formula with p terms we can reduce that error to $O(1/N^p)$.

3 General Properties of Path Integrals

In the functional formalism the quantum mechanical amplitude $A(a, b; T) = \langle b|e^{-T\hat{H}}|a\rangle$ is given in terms of a path integral which is simply the $N \to \infty$

limit of the $(N-1)$– fold integral expression

$$A_N(a,b;T) = \left(\frac{1}{2\pi\epsilon_N}\right)^{\frac{N}{2}} \int dq_1 \cdots dq_{N-1}\, e^{-S_N} . \tag{4}$$

The Euclidean time interval $[0,T]$ has been subdivided into N equal time steps of length $\epsilon_N = T/N$, with $q_0 = a$ and $q_N = b$. S_N is the naively discretized action of the theory. We focus on actions of the form

$$S = \int_0^T dt\, \left(\frac{1}{2}\dot{q}^2 + V(q)\right) \text{ , with } S_N = \sum_{n=0}^{N-1}\left(\frac{\delta_n^2}{2\epsilon_N} + \epsilon_N V_n\right) , \tag{5}$$

where $\delta_n = q_{n+1} - q_n$, $V_n = V(\bar{q}_n)$, and $\bar{q}_n = \frac{1}{2}(q_{n+1} + q_n)$. We use units in which $\hbar$ and particle mass equal 1.

The calculations we present turn out to be simplest in the mid-point prescription where the potential V is evaluated at $\bar{q}_n$. A more important freedom related to our choice of discretized action has to do with the possibility of introducing additional terms that explicitly vanish in the continuum limit. Actions with such additional terms will be called effective. For example, the term $\sum_{n=0}^{N-1} \epsilon_N\, \delta_n^2\, g(\bar{q}_n)$, where g is regular when $\epsilon_N \to 0$, does not change the continuum physics since it goes over into $\epsilon_N^2 \int_0^T dt\, \dot{q}^2\, g(q)$, i.e. it vanishes as ϵ_N^2. Such terms do not change the physics, but they do affect the speed of convergence. A systematic study of the relation between different discretizations of the same path integral will allow us to explicitly construct a series of effective actions with progressively faster convergence to the continuum. Before we do this we will briefly mention some general properties of the best effective action.

The amplitude $A(a,b;T)$ of some theory with action S satisfies

$$A(a,b;T) = \int dq_1 \cdots dq_{n-1} A(b, q_{n-1}; \epsilon_N) \cdots A(q_1, a; \epsilon_N) , \tag{6}$$

for all N. This general relation is a direct consequence of the linearity of states in a quantum theory. In analogy with ordinary integrals let us now suppose that there exists an effective action S^* that is equivalent to S (i.e that leads to the same continuum limit for all path integrals) with the additional property that its N-fold discretized amplitude $A_N^*(a,b;T)$ does not depend on N,

$$A_N^*(a,b;T) = A(a,b;T) \text{ , and } S_N^* = \sum_{n=o}^{N-1}\left(\frac{\delta_n^2}{2\epsilon_N} + \epsilon_N W_n^*\right) . \tag{7}$$

The equivalence of S and S^* implies that $W^* \to V(\bar{q})$ when ϵ_N and δ go to zero. The final general property of W^* follows from the reality of amplitudes in the Euclidean formalism. Using the hermiticity of the Hamiltonian we find $A(a,b;T) = A(a,b;T)^\dagger = \langle b|e^{-T\hat{H}}|a\rangle^\dagger = \langle a|e^{-T\hat{H}}|b\rangle = A(b,a;T)$. In terms of W^* this gives us

$$W^*(\delta_n, \bar{q}_n; \epsilon_N) = W^*(-\delta_n, \bar{q}_n; \epsilon_N) , \tag{8}$$

or, said another way, only even powers of δ_n are present in the expansion of W^*:

$$W^*(\delta_n, \bar{q}_n; \epsilon_N) = g_0(\bar{q}_n; \epsilon_N) + \delta_n^2\, g_1(\bar{q}_n; \epsilon_N) + \delta_n^4\, g_2(\bar{q}_n; \epsilon_N) + \dots \,. \quad (9)$$

All the functions g_k are regular in the $\epsilon \to 0$ limit. The link to the starting theory is now simply $g_0(\bar{q}_n; \epsilon_N) \to V(\bar{q}_n)$ as ϵ_N goes to zero.

4 Relation Between Different Discretizations

We start by studying the relation between the $2N$-fold and N-fold discretizations of the same theory. From eq. (4) we see that we can write the $2N$-fold amplitude as an N-fold amplitude given in terms of a new action $\widetilde{S}_N$ determined by

$$e^{-\widetilde{S}_N} = \left(\frac{2}{\pi\epsilon_N}\right)^{\frac{N}{2}} \int dx_1 \cdots dx_N\, e^{-S_{2N}}\,, \quad (10)$$

where S_{2N} is the $2N$-fold discretization of the starting action. We have written the $2N$-fold discretized coordinates $Q_0, Q_1, \dots, Q_{2N}$ in terms of q's and x's in the following way: $Q_{2k} = q_k$ and $Q_{2k-1} = x_k$.

Having in mind the results of the previous section, it is best to use the effective action which gives the same result for both the $2N$-fold and N-fold discretizations. Therefore, in this case we get

$$e^{-S_N^*} = \left(\frac{2}{\pi\epsilon_N}\right)^{\frac{N}{2}} \int dx_1 \cdots dx_N\, e^{-S_{2N}^*}\,. \quad (11)$$

From this one easily finds

$$\exp\left[-\epsilon_N W^*(\delta_n, \bar{q}_n; \epsilon_N)\right] = \\ = \left(\frac{2}{\pi\epsilon_N}\right)^{\frac{1}{2}} \int_{-\infty}^{+\infty} dy\, \exp\left(-\frac{2}{\epsilon_N} y^2\right) F\left(\bar{q}_n + y; \frac{\epsilon_N}{2}\right)\,, \quad (12)$$

where

$$-\frac{2}{\epsilon_N} \ln F(x; \epsilon_N) = g_0\Big(\frac{q_{n+1}+x}{2}; \epsilon_N\Big) + g_0\Big(\frac{x+q_n}{2}; \epsilon_N\Big) + \\ +(q_{n+1}-x)^2\, g_1\Big(\frac{q_{n+1}+x}{2}; \epsilon_N\Big) + (x-q_n)^2\, g_1\Big(\frac{x+q_n}{2}; \epsilon_N\Big) + \dots$$

The above integral equation can be solved for the simple cases of a free particle and a harmonic oscillator, and gives the well known results. Note however that for a general case the integral in eq. (12) is in a form that is ideal for an asymptotic expansion. The time step ϵ_N is playing the role of small parameter (in complete parallel to the role $\hbar$ plays in standard semi-classical, or loop, expansion). As is usual, the above asymptotic expansion is carried through by first Taylor expanding $F\left(\bar{q}_n + y; \frac{\epsilon_N}{2}\right)$ around $\bar{q}_n$ and then by doing the remaining Gaussian integrals. Assuming that $\epsilon_N < 1$ (i.e. $N > T$) we have

$$g_0(\bar{q}_n; \epsilon_N) + \delta_n^2\, g_1(\bar{q}_n; \epsilon_N) + \delta_n^4\, g_2(\bar{q}_n; \epsilon_N) + \dots = \\ = -\frac{1}{\epsilon_N} \ln\left[\sum_{m=0}^{\infty} \frac{F^{(2m)}\left(\bar{q}_n; \frac{\epsilon_N}{2}\right)}{(2m)!!} \left(\frac{\epsilon_N}{4}\right)^m\right]\,. \quad (13)$$

Note that $F^{(2m)}(x;\epsilon_N)$ denotes the corresponding derivative with respect to x. All that remains is to calculate these expressions using the definition of the function F and to expand all the g_k's around the mid-point $\bar{q}_n$. This is a straight forward though tedious calculation. In general, if we wish to expand the effective action to ϵ_N^p we need to evaluate only g_0 (up to ϵ_N^{p-1}) and the remaining $p-1$ functions g_k (up to ϵ_N^{p-1-k}).

Although the system of recursive relations for g_k's is non-linear, it is in fact quite easy to solve if we remember that the system itself was derived via an expansion in ϵ_N. Having this in mind we first write all the functions as expansions in powers of ϵ_N that are appropriate to the level p we are working at. The $p=3$ level solution equals

$$g_0 = V + \epsilon_N \frac{V''}{12} + \epsilon_N^2 \left[-\frac{V'^2}{24} + \frac{V^{(4)}}{240} \right], \; g_1 = \frac{V''}{24} + \epsilon_N \frac{V^{(4)}}{480}, \; g_2 = \frac{V^{(4)}}{1920}.$$

Note that W^* depends only on the initial potential V and its derivatives (as well as on ϵ_N). One can similarly calculate the effective action S^* to any desired level p. We denote the p level truncation of the effective action as $S^{(p)}$. $S^{(p)}$ has the property that its N-fold amplitudes deviate from the continuum expressions as $O(\epsilon_N^p)$

$$A(a,b;T) = A_N^{(p)}(a,b;T) + O(\epsilon_N^p)\,. \tag{14}$$

Comparing this to eq. (3) we see that we have just derived the generalization of the Euler summation formula to path integrals. Expressions for effective actions up to $p=10$ can be found on our web site [12].

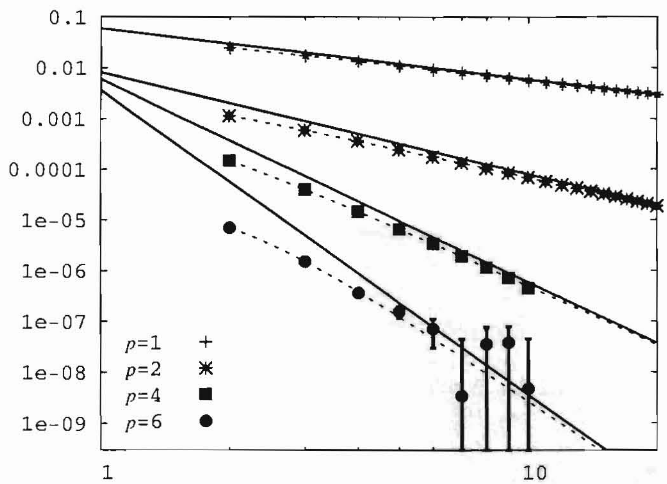

Figure 1. Deviations from the continuum limit $|A_N^{(p)} - A|$ as functions of N for $p = 1, 2, 4$ and 6 for an anharmonic oscillator with quartic coupling $\lambda = 10$, time of propagation $T = 1$ from $a = 0$ to $b = 1$, $N_{MC} = 9.2 \cdot 10^9$ for $p = 1, 2$, $9.2 \cdot 10^{10}$ for $p = 4$, and $3.68 \cdot 10^{11}$ for $p = 6$. Solid lines give the leading $1/N^p$ behavior.

We analyzed in detail several models: the anharmonic oscillator with quartic coupling $V = \frac{1}{2}q^2 + \frac{\lambda}{4!}q^4$ and a particle moving in a modified Pöschl-Teller potential over a wide range of parameters. In all cases we found agreement with eq. (14). Figure 1 illustrates this behavior in the case of an anharmonic oscillator. We see that the p level data indeed differs from the continuum amplitudes as a polynomial starting with $1/N^p$.

5 Conclusions

We have presented an algorithm that leads to significant speedup of numerical procedures for calculating path integrals. The increase in speed results from new analytical input that comes from a systematic investigation of the relation between discretizations of different coarseness and that leads to a generalization of the Euler summation formula to path integrals. We have presented an explicit procedure for obtaining a set of effective actions $S^{(p)}$ that have the same continuum limit as the starting action S, but which approach that limit ever faster. Amplitudes calculated using the N-point discretized effective action $S_N^{(p)}$ satisfy $A_N^{(p)}(a,b;T) = A(a,b;T) + O(1/N^p)$. We have obtained and analyzed the effective actions for $p \leq 10$ and have documented the speedup up to $1/N\,^10$ by conducting Monte Carlo simulations of several different models.

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