Institute of Physics, Belgrade
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Euler Summation Formula for Path Integrals

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Ordinary Integrals (1)

- Definition

$$I[f] \equiv \int_0^T f(t)dt = \lim_{N\to\infty} I_N[f]$$

$$I_N[f] = \sum_{n=1}^N f(t_n)\epsilon_N$$

$$\epsilon_N = T/N \qquad t_n = n\epsilon_N$$

- Bad for brute force numerical calculations

$$I_N[f] = I[f] + O(1/N)$$

Ordinary Integrals (2)

- To analytically solve even the simplest integrals you needed to:
  - Find useful discretization
  - Do general N-fold sum
  - Do the continuum limit
- Euler's summation formula
  - Speeds up convergence to the continuum limit as fast as you want
  - Wasn't of much use numerically – no computers in the 18th century
  - Pointed to an underlying simplicity – precursor to integration theory
- Riemmann's integration theory

Euler's formula (1)

- Discretization is not unique. Instead of $f(t)$ we construct an equivalent function $f^*(t;\epsilon_N)$:

$$f^*(t;\epsilon_N) \to f(t)$$ (in continuum limit)

such that

$$I_N[f^*] = I[f]$$ (for all N)

Euler's formula (2)

- Step 1: $f(t) = 1$

$$I_N[1] = \sum_{n=1}^{N} \epsilon_N = T$$

thus $f^* - f$ depends only on $\dot{f}, \ddot{f}, \ldots$

- Step 2: $f(t) = t$

$$I_N[t] = \sum_{n=1}^{N} t_n \epsilon_N = \frac{T^2}{2} + \frac{T^2}{2N}$$

$$I_N[t - \tfrac{\epsilon_N}{2}] = \frac{T^2}{2}$$

thus $f^* - f + \frac{\epsilon_N}{2}\dot{f}$ depends only on $\ddot{f}, \ldots$

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Euler's formula (3)

- Step 3: $f(t) = t^2$

$$I_N[t^2] = \sum_{n=1}^{N} t_n^2 \epsilon_N = \frac{T^3}{3} + \frac{T^3}{2N} + \frac{T^3}{6N^2}$$

$$I_N[t^2 - \epsilon_N t_n - \tfrac{2}{3}\epsilon_N^2] = \frac{T^3}{3}$$

thus $f^* = f - \frac{\epsilon_N}{2}\dot{f} - \frac{2\epsilon_N^2}{3}\ddot{f} + \ldots$

- etc.

Euler's formula (4)

- Therefore

$$\int_0^T f(t)dt = \sum_{n=1}^N f(t_n)\epsilon_N -$$

$$-\frac{\epsilon_N}{2}\sum_{n=1}^N \dot{f}(t_n)\epsilon_N - \frac{2\epsilon_N^2}{3}\sum_{n=1}^N \ddot{f}(t_n)\epsilon_N + \ldots$$

- We denote the first p terms of f^* by $f^{(p)}$. Then

$$I[f] = I_N[f^{(p)}] + O(1/N^p)$$

Path integrals (1)

- Amplitudes are the $N \to \infty$ limit of

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

- Action $S = \int_0^T dt\, \left(\frac{1}{2}\,\dot{q}^2 + V(q)\right)$

- Naïve discretized action

$$S_N = \sum_{n=0}^{N-1} \left(\frac{\delta_n^2}{2\epsilon_N} + \epsilon_N V_n\right)$$

$$\delta_n = q_{n+1} - q_n \qquad V_n = V(\bar{q}_n) \qquad \bar{q}_n = \frac{1}{2}(q_{n+1} + q_n)$$

Path integrals (2)

- Construct equivalent discretized effective action

$$S_N^* = \sum_{n=o}^{N-1} \left(\frac{\delta_n^2}{2\epsilon_N} + \epsilon_N W_n^* \right)$$

such that

$$A_N^*(a,b;T) = A(a,b;T)$$

- We first derive some general properties of W^*

Path integrals (3)

- All amplitudes may be written as

$$A(q_{n+1}, q_n; \epsilon_N) = \left(\frac{1}{2\pi\epsilon_N}\right)^{\frac{1}{2}} \exp\left(-\frac{\delta_n^2}{2\epsilon_N}\right) \mathcal{A}(q_{n+1}, q_n; \epsilon_N)$$

where $\mathcal{A} \to 1$ as $\epsilon_N \to 0$.

- Linearity of quantum states gives

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

- From this we find

$$\exp\left(-\epsilon_N W_n^*\right) = \mathcal{A}(q_{n+1}, q_n; \epsilon_N)$$

Path integrals (4)

- Although W_n^* is reminiscent of an effective potential it does not only depend on $\bar{q}_n$ but on δ_n and ϵ_N

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

- Reality of (Euclidean) amplitudes gives

$$A(a,b;T) = A(a,b;T)^\dagger =$$
$$= \langle b|e^{-T\hat{H}}|a\rangle^\dagger = \langle a|e^{-T\hat{H}}|b\rangle = A(b,a;T)$$

Path integrals (5)

- This implies

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

- Or, said another way

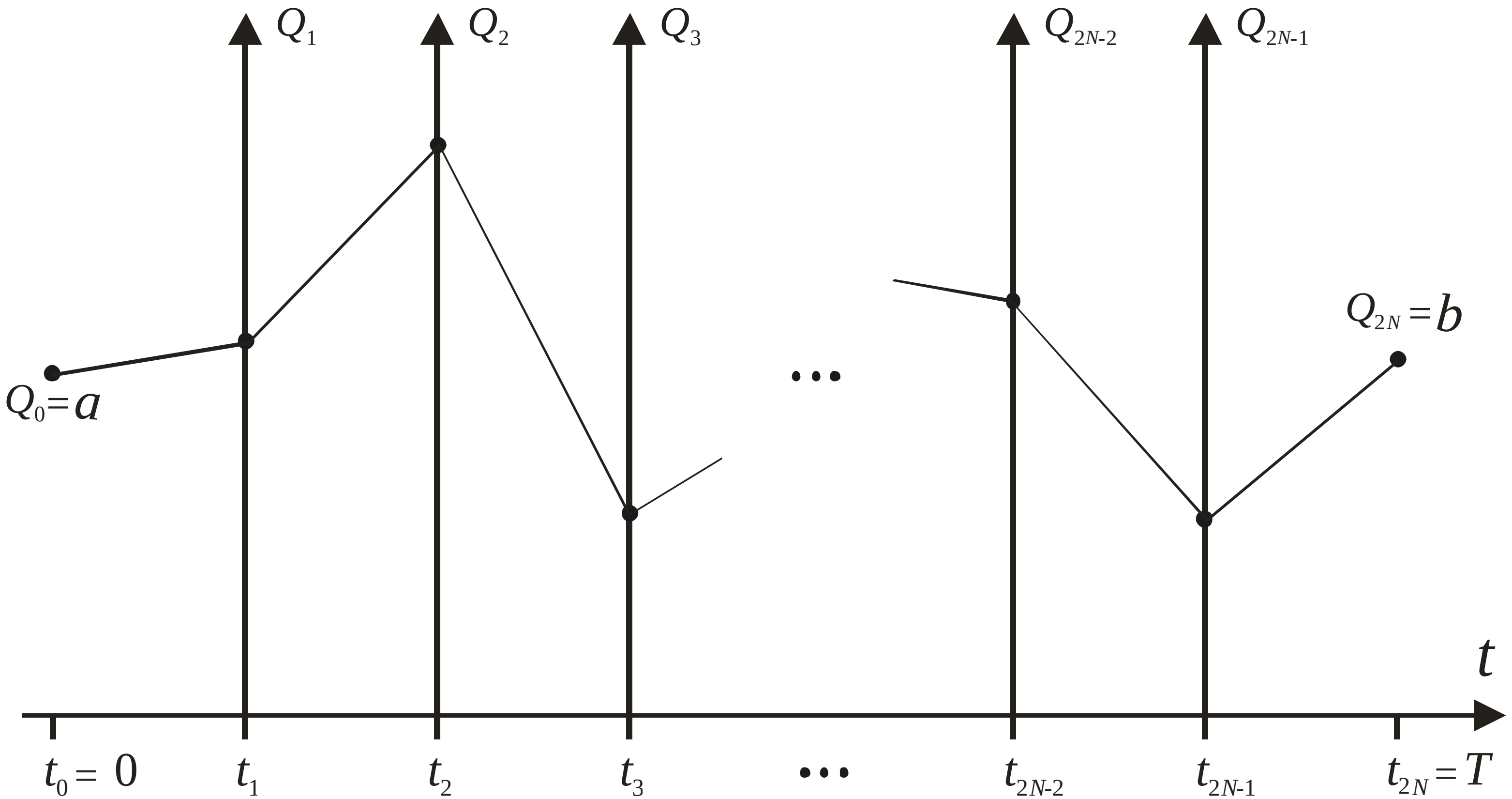
$$W^*(\delta_n, \bar{q}_n; \epsilon_N) =$$

$$= g_0(\bar{q}_n; \epsilon_N) + \delta_n^2\, g_1(\bar{q}_n; \epsilon_N) + \delta_n^4\, g_2(\bar{q}_n; \epsilon_N) + \ldots$$

All the g_k are regular in the continuum limit; also

$$g_0(\bar{q}_n; \epsilon_N) \to V(\bar{q}_n)$$

Compare discretizations (1)



Discretization with $2N$ time steps

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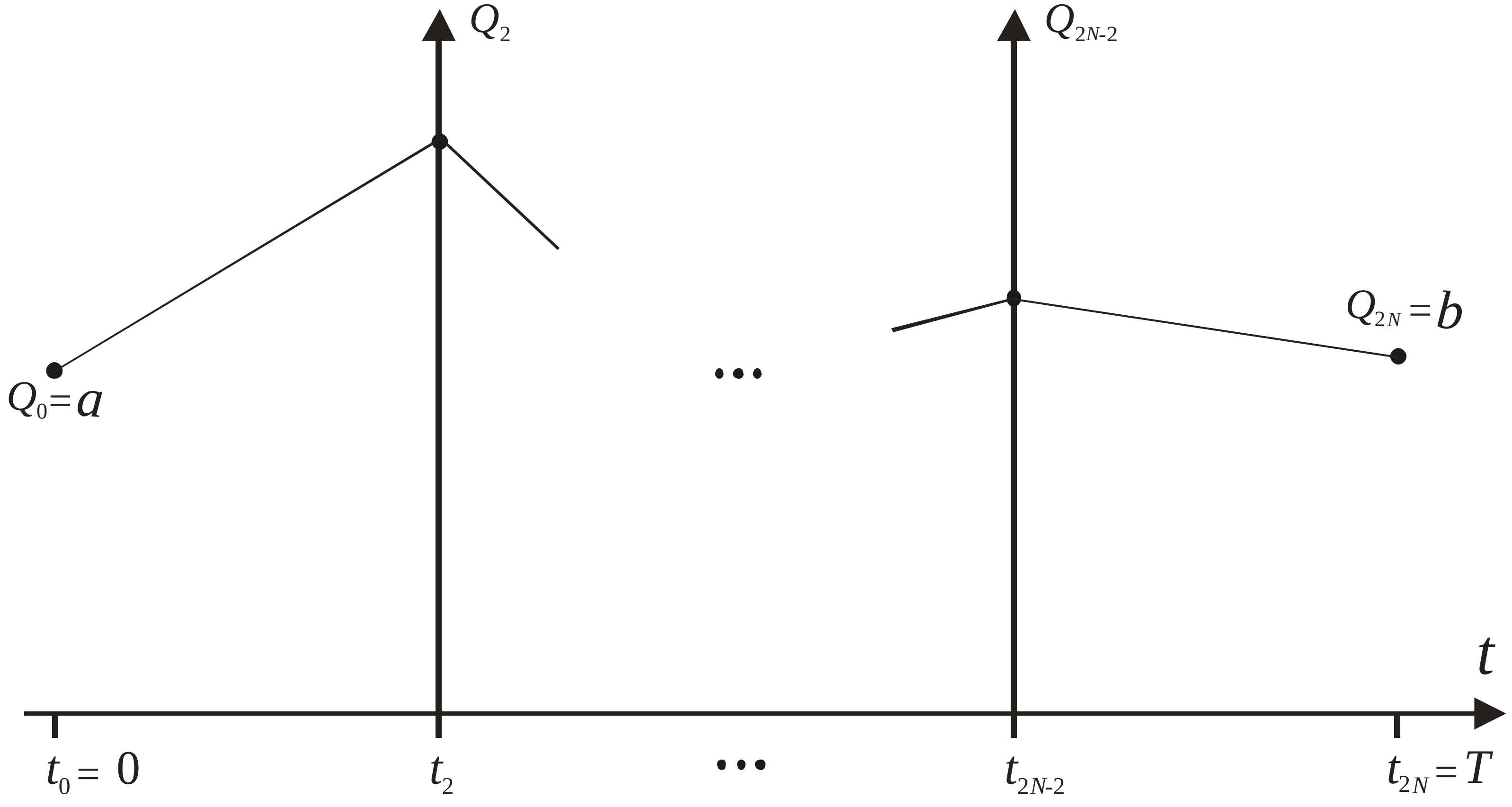
Compare discretizations (2)



Coarser discretization with N time steps

Compare discretizations (3)

- Integrating out every other point

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

- The $2N$-fold discretized coordinates $Q_0, Q_1, \ldots, Q_{2N}$ are given in terms of N-fold coordinates $q_0, q_1, \ldots, q_N$ and the intermediate points $x_1, x_2, \ldots, x_N$ according to $Q_{2k} = q_k$ and $Q_{2k-1} = x_k$

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Compare discretizations (4)

- N-fold amplitudes calculated with $\widetilde{S}$ give the same answer as $2N$-fold amplitudes calculated with S. If only we could actually do the integrals!
- Biggest problem: Even if we could integrate them once we couldn't iterate this procedure since $\widetilde{S}$ and S do not have the same functional form.
- Solution: use S^* (on both sides).

Compare discretizations (5)

- Get integral equation

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

where

$$-\frac{2}{\epsilon_N} \ln F(x; \epsilon_N) = g_0\left(\frac{q_{n+1} + x}{2}; \epsilon_N\right) + g_0\left(\frac{x + q_n}{2}; \epsilon_N\right) +$$
$$+ (q_{n+1} - x)^2 g_1\left(\frac{q_{n+1}+x}{2}; \epsilon_N\right) + (x - q_n)^2 g_1\left(\frac{x+q_n}{2}; \epsilon_N\right) + \ldots$$

- Works for free particle and harmonic oscillator. In general asymptotically expand - simpler than loop expansion. Small parameter is now ϵ_N

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Compare discretizations (6)

- Find

$$g_0(\bar{q}_n;\epsilon_N) + \delta_n^2\, g_1(\bar{q}_n;\epsilon_N) + \delta_n^4\, g_2(\bar{q}_n;\epsilon_N) + \ldots =$$

$$= -\frac{1}{\epsilon_N} \ln\left[\sum_{m=0}^{\infty} \frac{F^{(2m)}\left(\bar{q}_n;\frac{\epsilon_N}{2}\right)}{(2m)!!} \left(\frac{\epsilon_N}{4}\right)^m\right]$$

- All that remains is the tedious task of calculating all the derivatives and expanding all the g_k around the mid point $\bar{q}_n$ (easily done with a program like Mathematica). We have done this to level p=9, i.e. to $O(1/N^p)$

Compare discretizations (7)

- For example, to level $p=3$ we get

$$g_0(\bar{q}_n\,;\epsilon_N) = g_0\left(\bar{q}_n;\frac{\epsilon_N}{2}\right) + \epsilon_N\left[\frac{1}{4}g_1\left(\bar{q}_n;\frac{\epsilon_N}{2}\right) + \frac{1}{32}g_0''\left(\bar{q}_n;\frac{\epsilon_N}{2}\right)\right] +$$
$$+\epsilon_N^2\left[\frac{3}{16}g_2\left(\bar{q}_n;\frac{\epsilon_N}{2}\right) - \frac{1}{32}g_0'^{\,2}\left(\bar{q}_n;\frac{\epsilon_N}{2}\right) + \frac{1}{2048}g_0^{(4)}\left(\bar{q}_n;\frac{\epsilon_N}{2}\right) + \frac{3}{128}g_1''\left(\bar{q}_n;\frac{\epsilon_N}{2}\right)\right]$$

$$g_1(\bar{q}_n\,;\epsilon_N) = \frac{1}{4}g_1\left(\bar{q}_n;\frac{\epsilon_N}{2}\right) + \frac{1}{32}g_0''\left(\bar{q}_n;\frac{\epsilon_N}{2}\right) +$$
$$+\epsilon_N\left[\frac{3}{8}g_2\left(\bar{q}_n;\frac{\epsilon_N}{2}\right) + \frac{1}{1024}g_0^{(4)}\left(\bar{q}_n;\frac{\epsilon_N}{2}\right) - \frac{1}{64}g_1''\left(\bar{q}_n;\frac{\epsilon_N}{2}\right)\right]$$

$$g_2(\bar{q}_n\,;\epsilon_N) = \frac{1}{16}g_2\left(\bar{q}_n;\frac{\epsilon_N}{2}\right) + \frac{1}{6144}g_0^{(4)}\left(\bar{q}_n;\frac{\epsilon_N}{2}\right) + \frac{1}{128}g_1''\left(\bar{q}_n;\frac{\epsilon_N}{2}\right)$$

- The system was derived as an expansion in powers of ϵ_N . Expanding all the g_k appropriately we easily find the solution at the appropriate level p.

Compare discretizations (7)

- The level $p=3$ solution for S^* is

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

$$g_1 = \frac{V''}{24} + \epsilon_N \frac{V^{(4)}}{480}$$

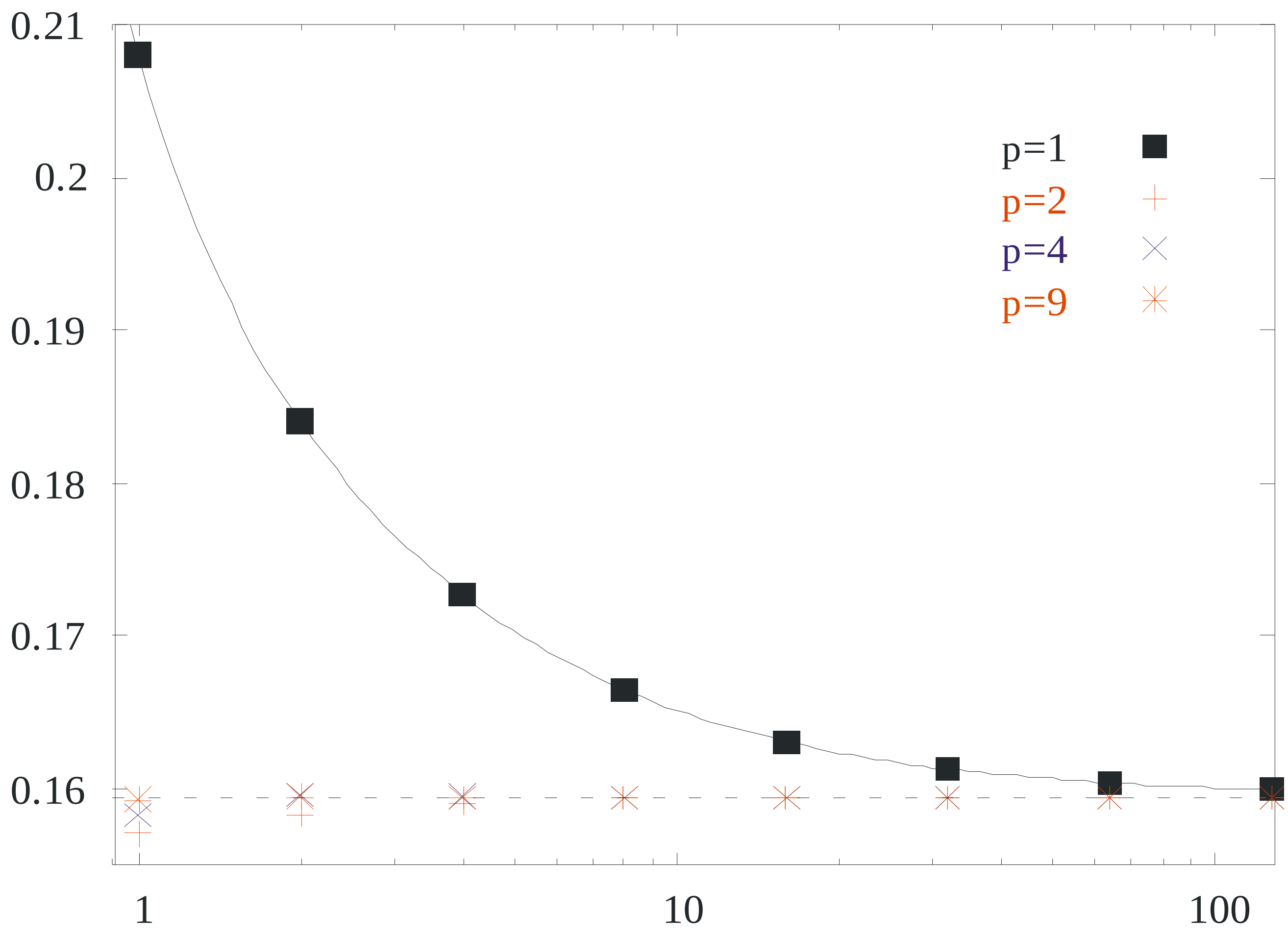
$$g_2 = \frac{V^{(4)}}{1920}$$

- Similarly for higher levels p. Note that the level p solution satisfies

$$A(a,b;T) = A_N^{(p)}(a,b;T) + O(1/N^p)$$

This is the Euler sum formula for path integrals.

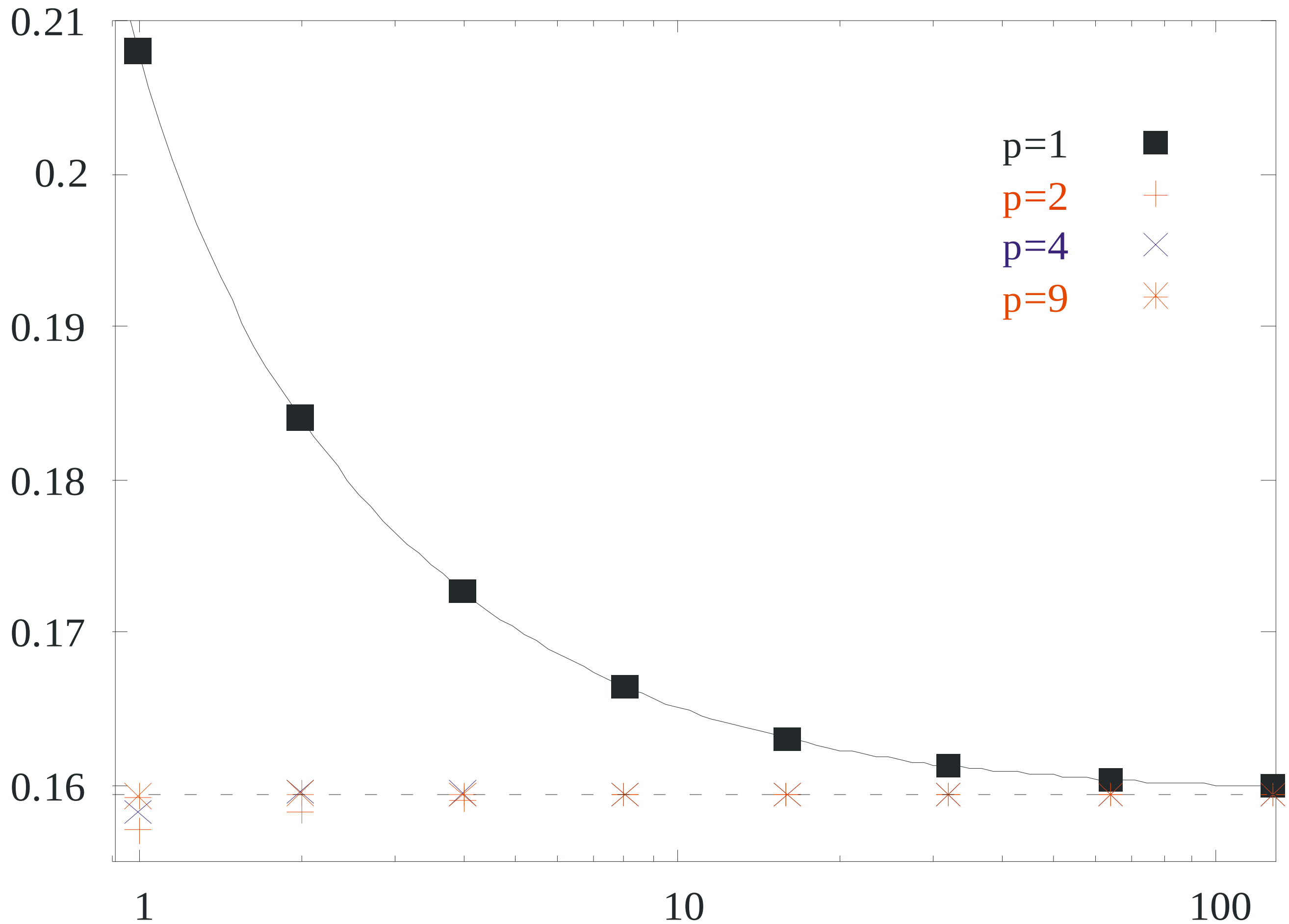
Numerical results (1)



Anharmonic oscillator with quartic coupling

$$g = 1,\ T = 1,\ a = 0,\ b = 1,\ N_{MC} = 10^7$$

Numerical results (2)



Modified Poeschl-Teller potential

$$\alpha = 0.5,\ \beta = 1.5,\ T = 1,\ a = 0,\ b = 1,\ N_{MC} = 9.2 \cdot 10^7$$

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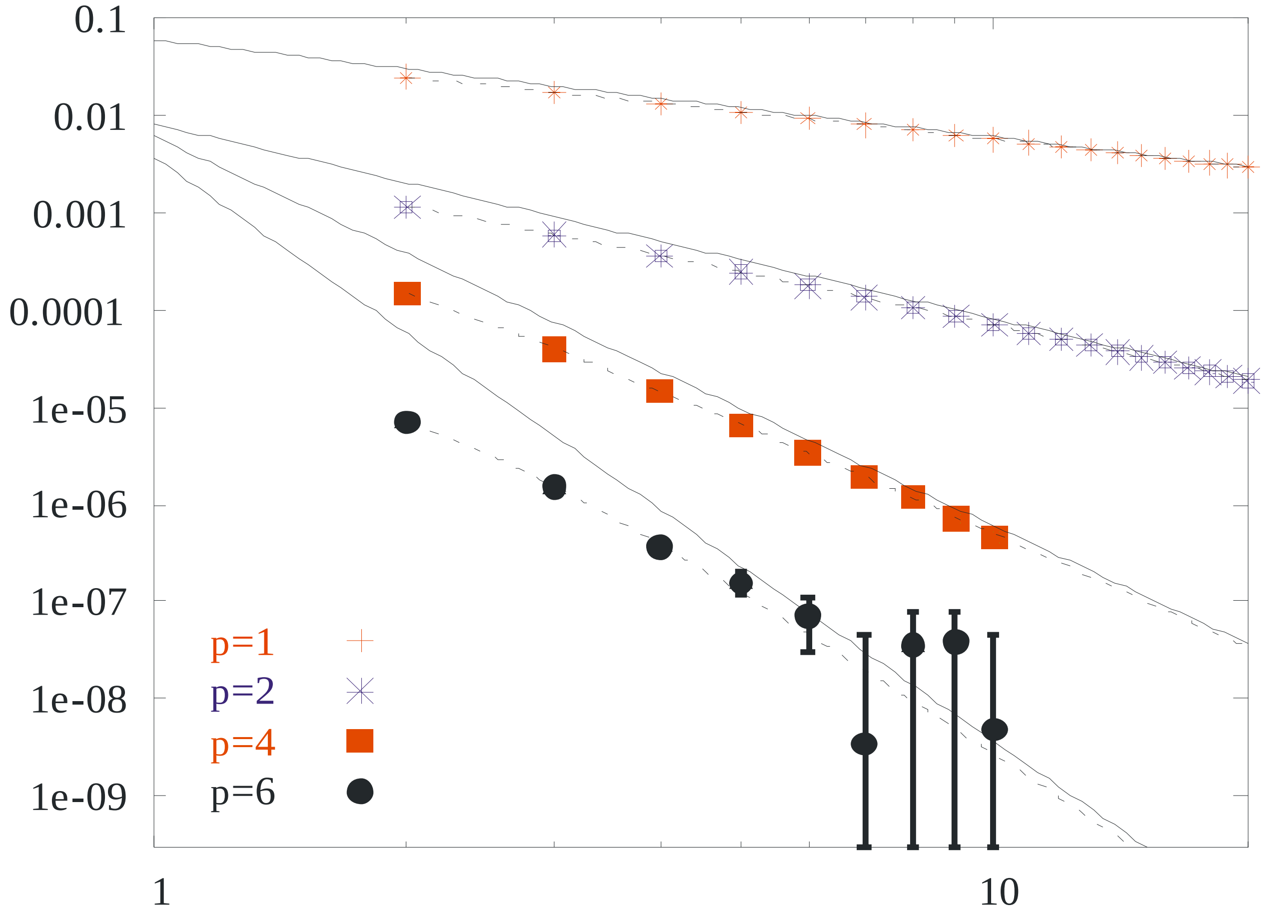
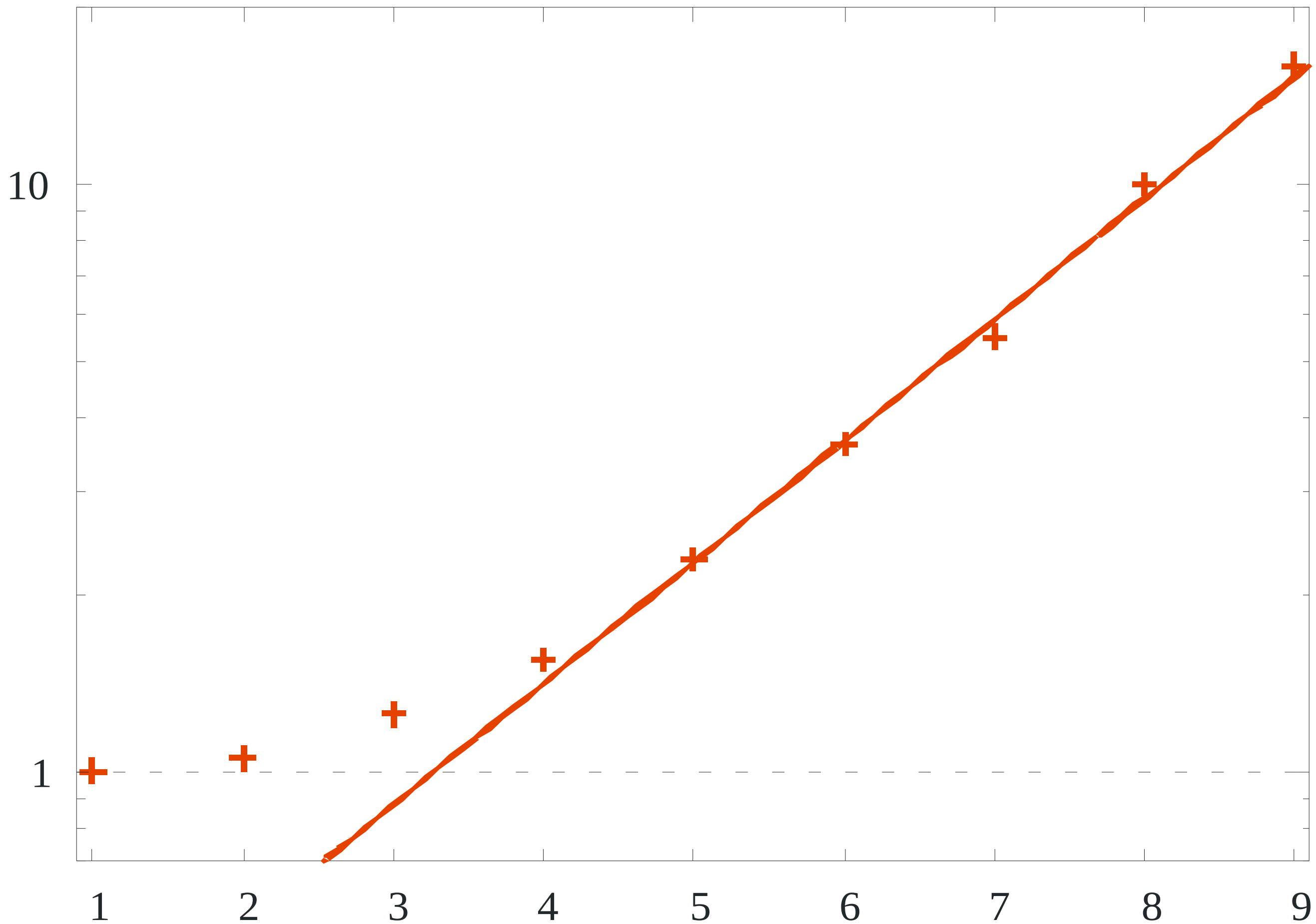
Numerical results (3)



Errors for anharmonic oscillator with quartic coupling

$$g = 1,\ T = 1,\ a = 0,\ b = 1,\ N_{MC} = 9.2 \cdot 10^9\ (p = 1, 2),$$
$$N_{MC} = 9.2 \cdot 10^{10}\ (p = 4),\ N_{MC} = 3.68 \cdot 10^{11}\ (p = 6)$$

Numerical results (4)



Relative increase in computing time as a function of p

Discussion (1)

- The general path integral calculation is now speeded up by many orders of magnitude.
- The same procedure works in Euclidean and Minkowski formalism (with appropriate $i\varepsilon$ prescription).
- The procedure has been checked on several different models across a wide range of parameters (in perturbative and non-perturbative regimes, across critical points, etc.)

Discussion (2)

- Extensions to many non-relativistic particles in d dimensions as well as to field theories in $d>1$ are in progress.
- Higher dimensional analogues of the integral equation are not a problem to derive. The asymptotic expansion procedure also works in all d. The algebraic recursive relations will be more complex and this could practically limit us to smaller values of p.

Highlights

- This is an analytic procedure that works for a generic model.
- The direct outcome of the procedure is a substantial speedup of numerical calculations of path integral (million fold or better).
- It now becomes possible to tackle complex models that could not be solved previously.
- An important outcome (not discussed in this presentation) are new analytical approximation techniques for path integrals.
- The true outcome of the work is heuristic – i.e. it leads to an increase of knowledge about path integration in general. It raises the hope that, as with ordinary integrals, the derivation of Euler's sum formula will be a precursor to the setting up of a general theory of path integration.

References

- A. Bogojević, A. Balaž and A. Belić, Phys. Rev. Lett. 94, 180403 (2005)
- A. Bogojević, A. Balaž and A. Belić, Submitted to Phys. Rev. B

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