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# Benchmarking Stochastic Techniques in Quantum Mechanics: Hunting for Excited States

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## Abstract

Standard Monte Carlo methods and Feynman Kac techniques to determine the quantum mechanical path integral are considered. Both methods are applied to isolate excited state eigenvalues.

# Benchmarking Stochastic Techniques in Quantum Mechanics: Hunting for Excited States

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## 1. Introduction

Many attempts have been made in recent years to compute excited hadronic states in lattice QCD (see e.g. [1]). The application of multi state variational techniques has been remarkably successful. The difficulty in the Euclidean approach to spectrum calculations is well known: the discrimination of subleading exponential terms against the leading ground state signal. Given this situation it appears to be rather helpful to illuminate the issue in the case of Quantum Mechanics. In this contribution, we will present a numerical analysis of the harmonic oscillator problem.

## 2. Correlator Method

Given an ensemble of quantum mechanical paths generated by a MC procedure, we calculate the correlation matrix

$$C_{lk}(\tau) = \langle (F_t^l - \langle F_t^l \rangle)\,(F_{t+\tau}^k - \langle F_{t+\tau}^k \rangle) \rangle \qquad (1)$$

consisting of all possible combinations of $N$ chosen observables $F^l$. In the long time limit the spectral decomposition of the correlation matrix has the form:

$$C_{lk}(\tau) = \sum_{n \neq 0} e^{-(\Delta E_n)\tau} \langle 0|F_t^l|n\rangle\langle n|F_t^k|0\rangle \qquad (2)$$

which contains the energy gaps $\Delta E_n$ of the system. Well chosen polynomials $F_l$ maximize the contribution of the first $N$ excitations and minimize the influence of higher ones in the correlation matrix.

We apply standard heatbath algorithm to produce 2000 quasi independent paths. Time resolution is set to $a = 0.015$ to avoid discretization errors. Each path consists of $2^{14}$ lattice points. The computational effort to generate the paths and measure $C_{lk}(\tau); F^l = x^l; N = 4; \tau \in [0,4]$ on a 8192 node CM2 is about 8 hours.

The analysis proceeds from the generalized eigenvalue problem

$$C_\tau u = \lambda(\tau, \tau_0) C_{\tau_0} u \qquad (3)$$

by diagonalizing the correlation matrix by [2]:

$$\lambda(\tau, \tau_0) \propto C_{\tau_0}^{-\frac{1}{2}} C_\tau C_{\tau_0}^{-\frac{1}{2}}. \qquad (4)$$

The procedure can be viewed as a generalization of the familiar local mass formalism to matrices. The energy gaps (Fig. 1) are computed by:

$$\Delta E_n = \ln\left(\frac{\lambda(\tau, \tau_0)}{\lambda(\tau + 4 * a, \tau_0)}\right). \qquad (5)$$

The reference time $\tau_0$ is taken as large as possible for the inversion of $C_{\tau_0}$ to remain stable. Within the statistical uncertainties we verify the lower eigenvalues to be stable under reducing $N$.

## 3. Feynman Kac Technique

In the spirit of Donsker and Kac [3] the functional integral is viewed as an expectation value based on an underlying *stochastic process* that gives rise to a characteristic functional measure. We will base our present work on the Wiener

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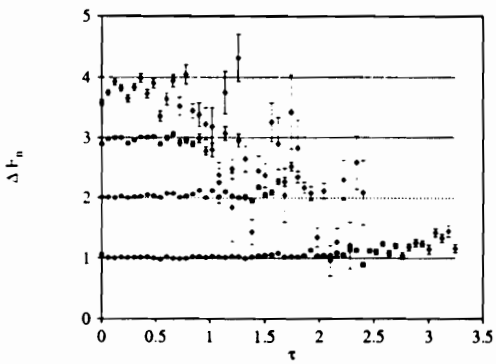


Figure 1. *Energy gaps for $\tau_0 = 0.5$. The solid lines are the theoretical expectations.*

process[2], which does not know the potential and thus can serve as a worst case study for the performance of the Feynman Kac approach.

The partition function can be written as an integral over an expectation value based on Brownian paths starting from $\omega(0) = x$ and ending at $\omega(t) = x'$ [4]:

$$Z(t) = \int \langle \exp\left(-\int_0^t ds\, V(\omega(s))\right) \delta_{x,x'} \rangle dx. \quad (6)$$

## 4. Updating Procedure

The evaluation of the stochastic functional in eq.(6) is performed on a spatial hypercubic lattice with lattice spacing $a = \sqrt{3dt}$. The Markov step

$$\begin{aligned} x_0 &= \omega(0) = x \quad (7) \\ x_{i+1}^k &= x_i^k + z_i^k, \quad k = 1, ..., d \end{aligned}$$

implies random numbers $z_i$ with probability

$$P(z_i = \pm\sqrt{3dt}) = \frac{1}{6}, \quad P(z_i = 0) = \frac{2}{3}. \quad (8)$$

These paths converge for small $dt$ to Brownian paths. The time integral in eq. 6 is estimated using:

$$I_{i+1} = I_i + \frac{dt}{2}\left(V(x_i) + V(x_{i+1})\right). \quad (9)$$

This discretization scheme is of order $(dt)^2$ and can be interpreted as generalization of the Simpson rule in the deterministic case. After each iteration step the expectation value

$$Z_{i+1}(x) = \langle \exp\left(-I_{i+1}\right)\delta_{x,x_{i+1}} \rangle \quad (10)$$

over all generated paths is calculated. This observable relates only to *cyclic* Brownian paths which decrease asymptotically in the number of iterations with $P(n) \propto \frac{1}{\sqrt{n}}$. The iteration is repeated with several initial locations $x_o = x$. To compute the partition function, $Z_{i+1}(x)$ is integrated over $x$.

In the numerical simulation we generate $33*2^{24}$ Brownian paths of time length $T = 7$, approximated with the time discretization $dt = 0.02$ to avoid discretization errors. We sample the starting points from the interval $x \in [-4, 4]$. The computational effort to generate the paths and calculate the partition function on a 8192 node CM2 is about 8 hours.

In the Feynman Kac approach the stochastic process generates paths in physical time. Different paths are entirely independent of each other, because no evolution in fictitious time is needed, unlike in standard MC techniques.

## 5. Spectral Analysis

The spectral decomposition of the partition function reads:

$$Z(t) = \int_{R^d} dx \langle x, 0|x, t\rangle = \sum_i \exp(-E_i t). \quad (11)$$

Many-parameter fits with $t' \in [t_{min}, t]$ of the form:

$$F(E_0, ..., E_n) = c \sum_{i=0}^{n_{max}} \exp(-E_i t') \quad (12)$$

are made to isolate the energies (c is an overall constant). Correlations in $t'$ are incorporated using bootstrap analysis. It is a crucial problem to specify the combination $t_{min}$ and the number $n_{max}$ for which the fit gives the most reliable and stable results. In order to get the best

[2] In the actual numerical simulations one improve by using more sophisticated stochastic processes, which are better adapted to the particular potential under consideration.

fit we vary the time cutoff $t_{min}$ and search for the best $\chi^2/dof$. $t_{min}$ controls the resolution of

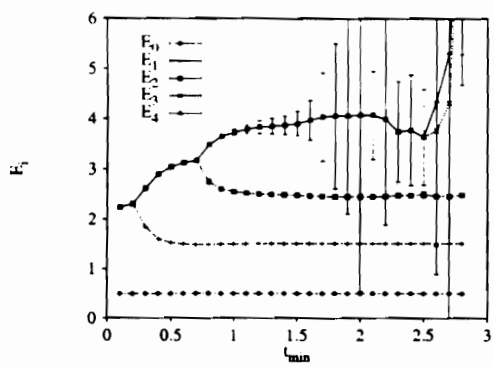


Figure 2. Fit results for $n_{max} = 5$ versus $t_{min}$. Minimum of $\chi^2/dof = 0.989$ is at $t = 1.7$. The theoretical values are $E_n = n + \frac{1}{2}$.

the highest excited states, as illustrated in Fig. 2 by a bifurcation-like structure of the "spectrum". The stability of the lowest lying results is verified by variation of $n_{max}$. The highest branch in Fig. 2 relates to two "unresolved" excited states, which we disentangle by a bootstrap histogram, as shown in Fig. 3. The histogram shows three maxima, which are hidden in Fig. 2. We hope that the knowledgeable reader will make out the 5th energy level.

## Conclusion

We applied correlator methods used in LGT in the quantum mechanical case in order to determine the spectrum. All difficulties which appear in the case of LGT find their analogy in the quantum mechanical situation, which acts as a fruitful playground to investigate and optimize analyzing methods.

Furthermore we provided a numerical procedure based on the stochastic formulation of pathintegrals which allows to simulate the full time development of the quantum mechanical

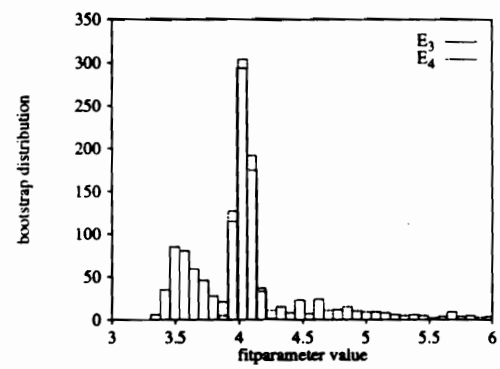


Figure 3. Histogram of $E_3$ and $E_4$ on each bootstrap. Time cutoff is set to $t_{min} = 1.7$.

partition function in Euclidean time. The analysis has been extended to the investigation of wave functions and more sophisticated underlying stochastic processes [5].

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