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Using a fermionic ensemble of systems to determine excited states

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Abstract

We discuss a new numerical method for the determination of excited states of a quantum system using a generalization of the Feynman–Kac formula. The method relies on introducing an ensemble of non-interacting identical systems with a fermionic statistics imposed on the systems as a whole, and on determining the ground state of this fermionic ensemble by taking the long-time limit of the Euclidean kernel. Due to the exclusion principle, the ground state of an n-system ensemble is realized by the set of individual systems occupying successively the n lowest states, all of which can therefore be sampled in this way. To demonstrate how the method works, we consider a one-dimensional oscillator and a chain of harmonically coupled particles.

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1. Introduction

A central object in the lattice formulation of field theory is the Euclidean kernel, which is obtained from the quantum amplitude by a Wick rotation. For a d-dimensional quantum field theory, the Euclidean kernel can be interpreted as a partition function for a $(d+1)$-dimensional classical statistical theory. This theory can then be put on a lattice and simulated by Monte Carlo methods.

The Euclidean kernel contains all the information about the quantum system, including in particular the excited states which in field theory correspond to particle states. Standard methods of extracting this information from numerical lattice data, commonly used for instance in QCD lattice spectroscopy, are based on the analysis of the long-time behaviour of the Euclidean kernel [1].

In this paper, we present a new method of determining excited states by studying the long-time behaviour of the Euclidean kernel for an ensemble of identical systems with a fermionic statistics. The trick of using a fermionic ensemble of systems allows us to subtract the contribution from the ground state and focus directly on the contribution from the lowest excited state. The method can be recursively extended to the next excited states.

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The first part of the paper contains standard material, which we recall here mainly to introduce the notation for the second part of the paper. In this second part, we discuss the new method and present results obtained from applying it to the cases of a single harmonic oscillator and of a one-dimensional chain of coupled particles.

We write most of our formulae in a quantum mechanical framework, which corresponds to a zero-dimensional ($d = 0$) quantum field theory. The generalization to ($d > 0$)-dimensional cases is straightforward and does not require a modification of the method or the underlying idea, although as we shall see some practical limitations occur in this case, which are related to the sign problem.

2. Standard methods

The Euclidean kernel is defined as

$$K_\tau(q_\mathrm{f}|q_\mathrm{i}) = \langle q_\mathrm{f}|\mathrm{e}^{-\tau H}|q_\mathrm{i}\rangle = \sum_{n=0} \phi_n^*(q_\mathrm{f})\phi_n(q_\mathrm{i})\ \mathrm{e}^{-\tau E_n} \tag{1}$$

where $\phi_n(q) = \langle q|n\rangle$ are eigenvectors of the Hamiltonian $H|n\rangle = E_n|n\rangle$ ordered by E_n, $E_0 \leqslant E_1 \leqslant \ldots$. The parameter τ is real and non-negative. We set $\hbar = 1$. The kernel can be expressed as a sum over paths propagating in time from an initial position q_i at some initial time τ_i to a final position q_f at some later time τ_f, $\tau = \tau_\mathrm{f} - \tau_\mathrm{i} \geqslant 0$ [2,3]. Using the composition rule

$$K_{\tau+\sigma}(q_\mathrm{f}|q_\mathrm{i}) = \int \mathrm{d}q\ K_\tau(q_\mathrm{f}|q)\ K_\sigma(q|q_\mathrm{i}) \tag{2}$$

and applying it many times to equal time intervals ϵ ($N\epsilon = \tau$), one finds

$$K_\tau(q_\mathrm{f}|q_\mathrm{i}) = \int \prod_{j=1}^{N-1} \mathrm{d}q_j \prod_{k=1}^{N} K_\epsilon(q_k|q_{k-1}) \tag{3}$$

where $q_\mathrm{f} = q_N$ and $q_\mathrm{i} = q_0$. As it stands, the formula (3) is of not much practical use, since the same unknown function K appears on both sides of the equation. The idea is now to use an approximation for small ϵ, replacing on the right-hand side K_ϵ with the semi-classical propagator $\mathcal{K}_\epsilon$. As an example, consider a quantum mechanical system with the Hamiltonian $H = p^2/2 + V(q)$, which describes a particle in D dimensions. Then the semi-classical propagator $\mathcal{K}_\epsilon$ is for small ϵ given by

$$\mathcal{K}_\epsilon(q_k|q_{k-1}) = (2\pi\epsilon)^{-D/2}\ \mathrm{e}^{-\epsilon\Delta S_k} \tag{4}$$

where

$$\Delta S_k = \frac{1}{2}\Big(\frac{q_k - q_{k-1}}{\epsilon}\Big)^2 + V(q_k). \tag{5}$$

Using this, we can approximate the kernel (3) for finite $\tau = N\epsilon$ by

$$K(q_\mathrm{f}|q_\mathrm{i}) \approx \int \prod_{j=1}^{N-1} \mathrm{d}q_j \prod_{k=1}^{N} \mathcal{K}_\epsilon(q_k|q_{k-1}) = \int Dq\ \mathrm{e}^{-S} \tag{6}$$

where

$$Dq = (2\pi\epsilon)^{-ND/2} \prod_{j=1}^{N-1} \mathrm{d}q_j = \mathcal{C} \prod_{j=1}^{N-1} \mathrm{d}q_j \qquad S = \epsilon \sum_{k=1}^{N} \Delta S_k. \tag{7}$$

For given N and ϵ, the factor $\mathcal{C}$ is just a global normalization. In the limit $N \to \infty$ with $\tau = N\epsilon = \text{const}$, the formula (6) approaches the exact one (3). Because the composition

rule (3) holds already before the Wick rotation is done, one can use formula (3) to perform calculations of the kernel directly in the real time. In this case one has to approximate the short time kernel by a finite matrix. It turns out, however, that this approximated matrix properly encodes the information about the lowest excited states [4].

The expression (6) can be viewed as a partition function for a classical field $\{q_j\}$ on a one-dimensional lattice, $j = 0, \ldots, N$, weighted by the exponent of the Euclidean action: $Dq\, \mathrm{e}^{-S}$. One can simulate such an ensemble of $\{q_j\}$ using standard Monte Carlo techniques. It is convenient to impose periodic boundary conditions, i.e. to set $q_0 = q_N = q$, and then to sum over q. The partition function for the ensemble of such periodic chains is

$$Z = \int \prod_{j=1}^{N} \mathrm{d}q_j \prod_{k=1}^{N} \mathcal{K}_\epsilon(q_k|q_{k-1}) = \int_{\text{periodic } q} Dq\, \mathrm{e}^{-S}. \tag{8}$$

This function serves as an approximation of the quantum mechanical expression

$$\int \mathrm{d}q\; K_\tau(q|q) = \int \mathrm{d}q\; \mathrm{e}^{-\tau E_0}\big\{|\phi_0(q)|^2 + |\phi_1(q)|^2 \mathrm{e}^{-\tau(E_1-E_0)} + \cdots\big\}. \tag{9}$$

On the one hand, the integrand $\mathrm{d}q\, K_\tau(q|q)$ corresponds to the probability distribution of positions q in the quantum system, but on the other hand it also describes the probability distribution of particle positions q_k in the ensemble of classical chains. For each particle of the chain the distribution is the same because the partition function is translationally invariant. In the large-τ limit, the integrand $\mathrm{d}q\, K_\tau(q|q) \to \mathrm{d}q\, \mathrm{e}^{-\tau E_0}|\phi_0(q)|^2$ is dominated by the contribution from the ground state. This is commonly known as the Feynman–Kac formula. The distribution of particle positions can be measured in Monte Carlo simulations of the classical chains. This can serve as a practical method for determining the ground state $|\phi_0(q)|^2$ of the quantum system.

In the same way, one can also measure the energy of the ground state. For each time slice k define an estimator of the classical energy: $E_k = T_k + V_k$, where $V_k = V(q_k)$ and T_k denote the potential and kinetic parts, respectively. The matrix elements of the squared momentum p^2 are given by $(q_{k+1} - q_k)(q_k - q_{k-1})/\epsilon^2$; therefore, the kinetic energy T_k depends in principle on three time slices. However, we can also introduce a one-slice operator for T_k by making use of the virial theorem, which tells us that on average $\langle T_k\rangle = \frac{1}{2}\langle q_k V'(q_k)\rangle$. The operator on the right-hand side, $q_k V'(q_k)$, is a one-slice operator and so, with these definitions, is now E_k.

Denote the average over paths weighted by (8) by $\langle\cdots\rangle$. The average $\langle E_k\rangle$ does not depend on k, so we can average over slices $E = \frac{1}{N}\sum_k E_k$ to obtain an estimator with a smaller statistical error. In the large-τ limit,

$$\langle E\rangle = E_0 + (E_1 - E_0)\mathrm{e}^{-\tau(E_1-E_0)} + \cdots \tag{10}$$

approaches the ground-state energy E_0. Since the average on the left-hand side can be measured in the ensemble of chains, we thus have a method for computing E_0.

In the MC simulations one is restricted to chains of finite length N. In order to increase $\tau = N\epsilon$ for finite N, one has to increase ϵ. This introduces systematic errors since the deviations between K_ϵ and $\mathcal{K}_\epsilon$ grow with ϵ. Moreover, a small deviation from K_ϵ may accumulate and become amplified in the convolution of N such factors in the time interval $\tau = N\epsilon$ (6). This error can be reduced by including higher-order corrections in ϵ to $\mathcal{K}_\epsilon$ (4) by replacing the action (5) with a sort of improved action [5]:

$$\Delta S_k \to \Delta S_k^{\text{impr}} = \Delta S_k + \tfrac{1}{24}\epsilon^2 (V'(q_k))^2 + \cdots \tag{11}$$

which can be obtained by introducing higher-order corrections from the Baker–Campbell–Hausdorff formula in the semi-classical approximation (4). One can now make an optimal

choice of N and ϵ so as to balance the systematic and statistical errors. As it stands, the method may be applied only to the ground state since the contributions from higher states in (9) and (10) are exponentially suppressed.

To determine the first excited state from the path integral approach, one has to remove the leading contribution. In the standard method this is done by calculating connected correlation functions for two different time slices k_a and k_b that are separated by a time interval $\Delta\tau = \tau_b - \tau_a = \epsilon(k_b - k_a)$. For any one-slice operator $\mathcal{O}$ one measures the correlation function $\langle \mathcal{O}(\tau_a)\mathcal{O}(\tau_b)\rangle$ in the ensemble of chains, which is related to the following expression in the quantum system:

$$\langle \mathcal{O}(\tau_a)\mathcal{O}(\tau_b)\rangle = \frac{1}{Z}\sum_{m,n} \mathrm{e}^{-(\tau-\Delta\tau)E_m}\langle m|\mathcal{O}|n\rangle \mathrm{e}^{-\Delta\tau E_n}\langle n|\mathcal{O}|m\rangle. \tag{12}$$

In the limit of large τ, i.e. $\tau \gg \Delta\tau$, only the contribution from the ground state $|m\rangle = |0\rangle$ survives in the sum. One obtains in this limit

$$\langle \mathcal{O}(\tau_a)\mathcal{O}(\tau_b)\rangle = \sum_{n=0}^{\infty} \left|\langle 0|\mathcal{O}|n\rangle\right|^2 \mathrm{e}^{-\Delta\tau(E_n - E_0)}. \tag{13}$$

The first term in the sum, $|\langle 0|\mathcal{O}|0\rangle|^2$, is independent of $\Delta\tau$ and can be subtracted by calculating the connected correlator:

$$\langle\!\langle \mathcal{O}(\tau_a)\mathcal{O}(\tau_b)\rangle\!\rangle = \langle \mathcal{O}(\tau_a)\mathcal{O}(\tau_b)\rangle - \langle \mathcal{O}(\tau_a)\rangle\langle \mathcal{O}(\tau_b)\rangle. \tag{14}$$

For large $\Delta\tau$ this is dominated by

$$\langle\!\langle \mathcal{O}(\tau_a)\mathcal{O}(\tau_b)\rangle\!\rangle = |\langle 0|\mathcal{O}|1\rangle|^2 \mathrm{e}^{-\Delta\tau(E_1 - E_0)} + \cdots. \tag{15}$$

Thus, the difference $E_1 - E_0$ can be numerically determined by measuring the exponential fall-off of the correlation function (15) for large $\Delta\tau$. The freedom one has in choosing the operator $\mathcal{O}$ should be used in practice to maximize the coefficent $|\langle 0|\mathcal{O}|1\rangle|^2$ relative to the coefficients for higher states $n > 2$.

It is clear from the discussion above that this method requires a large separation of timescales $0 \ll \Delta\tau \ll \tau$. This is a strong practical restriction. Moreover, computations of connected correlation functions are in general much more time consuming than calculations of averages. An additional difficulty arises from the fact that the signal-to-noise ratio is usually very small in the region of large $\Delta\tau$, where one has to carry out measurements of the exponential fall-off coefficient, $E_1 - E_0$.

To summarize, this method is much more demanding in computer power than the procedure for determining the energy of the ground state that we described before.

3. Antisymmetrization over systems

We now propose another way of subtracting the contribution from the ground state. We first consider an ensemble consisting of two non-interacting identical systems, with a fermionic statistics imposed on the systems as a whole. The Pauli principle then forbids the two individual systems to be in the same state simultaneously. Thus, the ground state of the ensemble corresponds to one of the sub-systems being in its ground state and the other one occupying the lowest excited state.

Denote the two systems by Q and R. They are independent and indistinguishable. Impose the fermionic statistics on them by defining the propagator for the twin system, $\hat{K}^{(2)}$, as the antisymmetrization of the individual propagators:

$$\hat{K}^{(2)}_\tau(q_\mathrm{f}, r_\mathrm{f}|q_\mathrm{i}, r_\mathrm{i}) = \frac{1}{2!}\left\{K_\tau(q_\mathrm{f}|q_\mathrm{i})K_\tau(r_\mathrm{f}|r_\mathrm{i}) - K_\tau(r_\mathrm{f}|q_\mathrm{i})K_\tau(q_\mathrm{f}|r_\mathrm{i})\right\}. \tag{16}$$

It follows from (2) that this function fulfills the same kind of composition rule:

$$\hat{K}^{(2)}_{\tau+\sigma}(q_{\rm f}, r_{\rm f}|q_{\rm i}, r_{\rm i}) = \int {\rm d}q\ {\rm d}r\ \hat{K}^{(2)}_{\tau}(q_{\rm f}, r_{\rm f}|q, r)\hat{K}^{(2)}_{\sigma}(q, r|q_{\rm i}, r_{\rm i}). \tag{17}$$

Thus, we can repeat the same approximation scheme as for the individual propagators (6). We obtain

$$\hat{K}^{(2)}_{\tau}(q_{\rm f}, r_{\rm f}|q_{\rm i}, r_{\rm i}) \approx \int \prod_{j=1}^{N-1} {\rm d}q_j\ {\rm d}r_j \prod_{k=1}^{N} \hat{\mathcal{K}}^{(2)}_{\epsilon}(q_k, r_k|q_{k-1}, r_{k-1}) \tag{18}$$

where

$$\hat{\mathcal{K}}^{(2)}_{\epsilon}(q_k, r_k|q_{k-1}, r_{k-1}) = \frac{1}{2!}\{\mathcal{K}_{\epsilon}(q_k|q_{k-1})\mathcal{K}_{\epsilon}(r_k|r_{k-1}) - \mathcal{K}_{\epsilon}(r_k|q_{k-1})\mathcal{K}_{\epsilon}(q_k|r_{k-1})\}\,. \tag{19}$$

Now we can define the partition function for the QR ensemble with periodic boundary conditions, analogously to (8). The partition function is related to the underlying quantum mechanical quantities as follows:

$$\begin{aligned}\hat{Z}^{(2)} &= \int {\rm d}q\ {\rm d}r\ \hat{K}^{(2)}_{\tau}(q, r|q, r) \\ &= \int {\rm d}q\ {\rm d}r\ {\rm e}^{-\tau\hat{E}^{(2)}_0}\left\{|\hat{\Phi}^{(2)}_0(q, r)|^2 + |\hat{\Phi}^{(2)}_1(q, r)|^2{\rm e}^{-\tau(\hat{E}^{(2)}_1 - \hat{E}^{(2)}_0)} + \cdots\right\} \\ &\to {\rm e}^{-\tau\hat{E}^{(2)}_0}\int {\rm d}q\ {\rm d}r\ |\hat{\Phi}^{(2)}_0(q, r)|^2\end{aligned} \tag{20}$$

where now $\hat{\Phi}^{(2)}_k(q, r)$ are wavefunctions of the twin system and $\hat{E}^{(2)}_k$ are the corresponding energy levels. The wavefunctions are constructed as Slater determinants of the wavefunctions of the individual systems. In particular, the ground state is $\hat{\Phi}^{(2)}_0(q, r) = \frac{1}{\sqrt{2!}}\{\phi_0(q)\phi_1(r) - \phi_1(q)\phi_0(r)\}$, and its energy is given by $\hat{E}^{(2)}_0 = E_0 + E_1$. This provides us with a practical method of determining the lowest excited state $|\phi_1(q)|^2$ and the corresponding energy E_1. The probability distribution of positions in one of the two systems, $P^{(2)}(q)$, can be expressed in terms of the wavefunctions of the individual system:

$$P^{(2)}(q) = \int {\rm d}r\ |\hat{\Phi}^{(2)}_0(q, r)|^2 = \tfrac{1}{2}\left\{|\phi_0(q)|^2 + |\phi_1(q)|^2\right\}. \tag{21}$$

Both $P^{(2)}(q)$ and $P^{(1)}(q) = |\phi_0(q)|^2$ can be measured numerically using the MC method, and we can put them together to find

$$|\phi_1(q)|^2 = 2P^{(2)}(q) - P^{(1)}(q). \tag{22}$$

Similarly, by subtracting the ground-state energy E_0 of an individual system from the ground-state energy $\hat{E}^{(2)}_0$ of the twin system we can determine the energy $E_1 = \hat{E}^{(2)}_0 - E_0$ of the first excited state of the individual system.

This method can be extended recursively to determine higher excited states as well. Namely, the energy E_k of the kth excited state can be computed as $E_k = \hat{E}^{(k+1)}_0 - \hat{E}^{(k)}_0$, the difference of the ground-state energies of the ensembles composed of k and $k-1$ antisymmetrized copies of the individual system, respectively. Similarly, for the kth excited state,

$$|\phi_k(q)|^2 = (k+1)P^{(k+1)}(q) - kP^{(k)}(q) \tag{23}$$

where $P^{(k)}$ is an appropriately normalized probability distribution

$$P^{(k)}(q) = \int |\hat{\Phi}^{(k)}_0(q, r, s, \ldots)|^2\,{\rm d}r\,{\rm d}s\ldots \tag{24}$$

for the ensemble of k antisymmetrized copies. In the Monte Carlo simulations of the ensemble of k copies, the probability distribution $P^{(k)}(q)$ is measured straightforwardly as a probability distribution of particle positions q in one of the k copies.

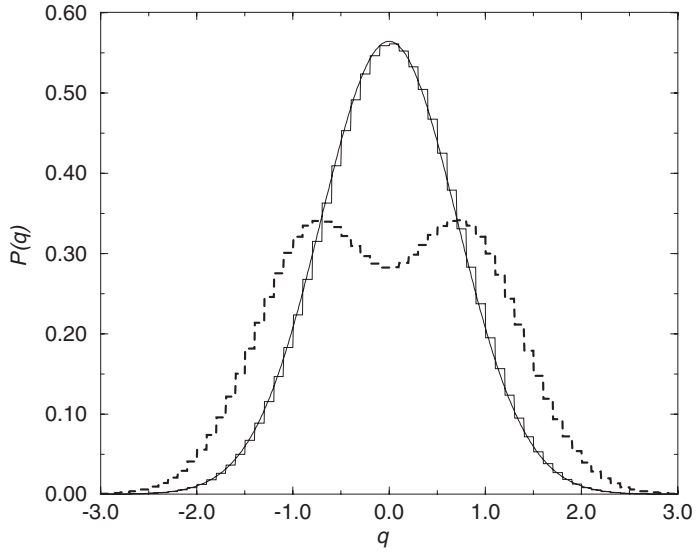

Figure 1. The histograms show the numerical results for $P_2(q)$ and $P_1(q)$ from the MC simulations. The solid curve represents the theoretical curve $|\phi_0(q)|^2$.

4. Results

Let us first illustrate how this method works for the one-dimensional harmonic oscillator: $V(q) = q^2/2$. In figure 1 we show the probability distributions $P^{(1)}(q) = |\phi_0(q)|^2$ and $P^{(2)}(q)$ in simulations with a single system and with the ensemble of two antisymmetrized copies, for $N = 128$ and $\epsilon = 0.0625$ (corresponding to $\tau = 8$). The solid curve going through the data points of $P^{(1)}(q)$ is given by the ground-state function of the oscillator: $|\phi_0(q)|^2 = \frac{1}{\sqrt{\pi}}\mathrm{e}^{-q^2}$. The difference between the two numerically obtained curves $2P^{(2)}(q) - P^{(1)}(q)$ is shown in figure 2, where it is compared to the function $|\phi_1(q)|^2 = \frac{2}{\sqrt{\pi}}q^2\mathrm{e}^{-q^2}$, which describes the first excited state squared of the oscillator. The agreement is perfect.

Physically, the appearance of the valley in the $P^{(2)}(q)$ distribution results from the fermionic repulsion between the two systems. The difference $|\phi_1(q)|^2 = 2P^{(2)}(q) - P^{(1)}(q)$ leads to a zero value of the probability.

The measured values of the energy of the ground state are $E_0 = 0.501(3)$ and $E_0^{(2)} = 2.006(6)$, which gives $E_1 = 1.505(7)$ in agreement with $E_n = n + \frac{1}{2}$.

The method also works very well for higher excited states. As an example we show, in figure 3, the probability distributions $P^{(4)}(q)$ and $P^{(3)}(q)$ and, in figure 4, the difference $4P^{(4)}(q) - 3P^{(3)}(q)$. The resulting curve is compared to the function $|\phi_3(q)|^2 = \frac{1}{2^3 3!}\frac{1}{\sqrt{\pi}}H_3^2(q)\mathrm{e}^{-q^2}$, where $H_3(q) = 8q^3 - 12q$ is the third Hermite polynomial, drawn as a solid line. Again, the agreement is very good.

As a second example, consider now a one-dimensional chain of harmonically coupled particles with the Hamiltonian

$$H = \sum_j^n \left[\frac{1}{2}p_j^2 + \frac{1}{2\varepsilon^2}(q_j - q_{j-1})^2 + V(q_j)\right]. \tag{25}$$

The index j runs over positions in the chain. The harmonic coupling constant between neighbours is $1/\varepsilon^2$. As before, using the path integral formulation we first write the kernel as a

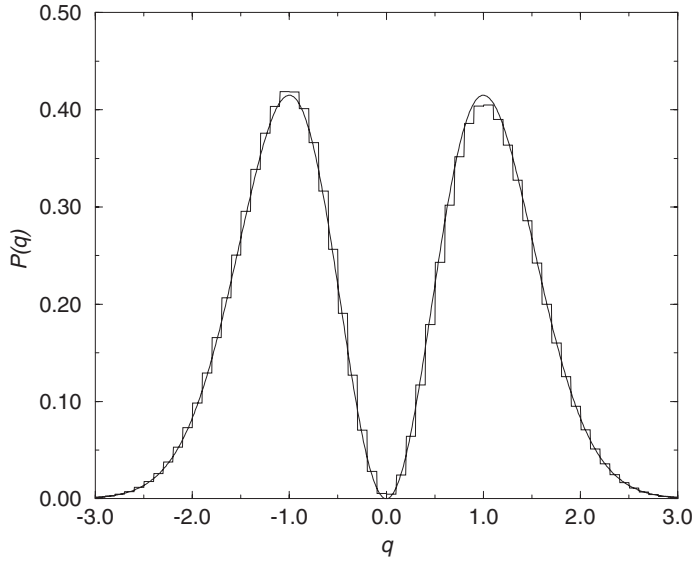

Figure 2. The histogram shows the normalized difference $2P_2(q) - P_1(q)$ of the data from figure 1. The solid curve represents the theoretical curve $|\phi_1(q)|^2$.

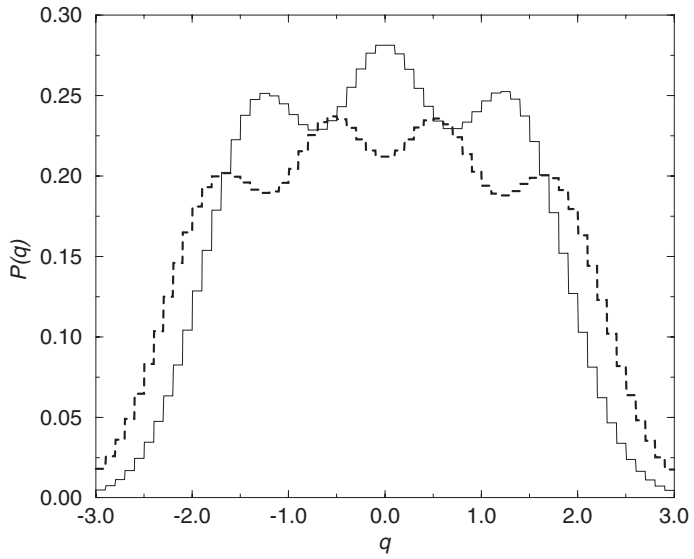

Figure 3. Numerical results for $P_4(q)$ and $P_3(q)$.

convolution of N propagators (3), and then approximate $K_\epsilon \to \mathcal{K}_\epsilon$ in the limit $\epsilon \to 0$. Similarly to (6), we obtain a classical partition function for the ensemble of fields $q_{k,j}$, distributed now on a two-dimensional lattice and weighted by the action

$$S_E = \sum_{(k,j)} \frac{1}{2}\left(\frac{q_{k+1,j} - q_{k,j}}{\epsilon}\right)^2 + \frac{1}{2}\left(\frac{q_{k,j+1} - q_{k,j}}{\varepsilon}\right)^2 + V(q_{k,j}) \tag{26}$$

with the integration measure $\sim \prod \mathrm{d}q_{k,j}$ (6), where the index k runs over time slices. Note

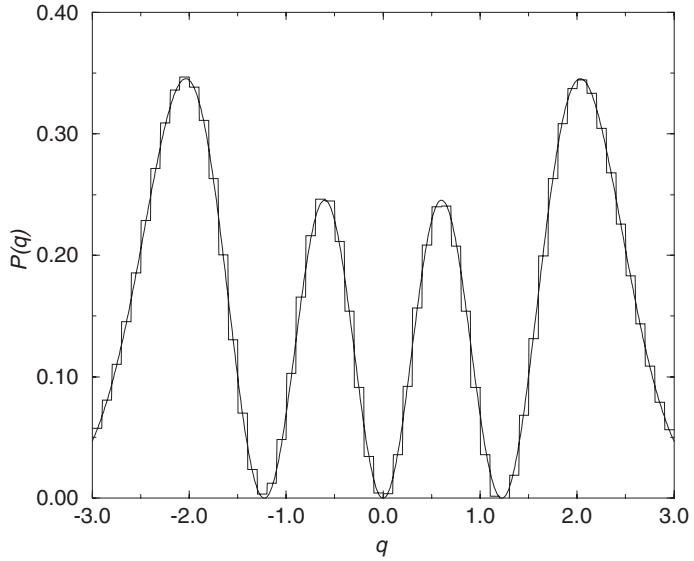

Figure 4. The normalized difference $4P_4(q) - 3P_3(q)$ of the data from figure 3. The solid curve represents the theoretical curve $|\phi_3(q)|^2$.

that despite the apparent similarity, the two parameters ϵ and ε have a different meaning: the former is a time-slicing parameter, whereas the latter is a harmonic constant of the chain.

One way of looking at the chain is from a quantum mechanical perspective. In this case one fixes the harmonic constant ε and for given τ makes the time-slicing dense, $N \to \infty$ and $\epsilon = \tau/N \to 0$. Alternatively, one can adopt a field-theoretical viewpoint by re-interpreting the parameter ε as a spatial lattice constant and keeping it proportional to ϵ: $c = \varepsilon/\epsilon = \text{const}$. In this case, the pair (k, j) can be viewed as a spacetime index. In the naive continuum limit $\epsilon \to 0$, the two terms in the sum (26) become a Lorentz (rotationally) invariant expression $(\partial_t q)^2 + c^2(\partial_x q)^2$, and therefore so does the whole theory. Thus, the expression (26) can be regarded as a discretization of the Euclidean action of a field theory, and the partition function as the Euclidean kernel of a quantum field theory. We see that the prescription for the quantization of the theory is almost the same as in quantum mechanics. It is commonly treated as a non-perturbative definition of quantum field theory.

A difference between quantum mechanics and field theory appears, however, when one wants to introduce the ϵ corrections. The formula (11), which works for quantum mechanics, does not work for quantum field theory since it breaks the symmetry between space and time. For quantum field theory one therefore has to use a different scheme (an 'improved action') to introduce lattice spacing corrections to the action which preserve the Lorentz invariance of the underlying continuum theory [6].

Here we will consider only the simplest case, namely a quantum chain with the potential $V(q) = q^2/2$, which we simulate on a periodic $(1 + 1)$-dimensional lattice with N nodes in the temporal direction and n in the spatial one. To each node we assign an appropriate particle displacement q.

The spectrum of this simple Hamiltonian is known. For convenience, we will write formulae only for odd $n = 2A + 1$. The Hamiltonian can be diagonalized in the Fourier modes Q_α, $\alpha = 0, 1, \ldots, A$. The modes for $\alpha > 0$ are twice degenerate, each having a left mover

Table 1. The mass gap m for various N and n ($\tau = 5$, $\varepsilon = 1$).

N	$n = 1$	2	3	5	7
16	0.981(3)		0.967(2)		
32	1.001(3)		0.993(4)		
64	1.001(3)	0.998(2)	1.001(7)	1.00(5)	1.04(7)
128	0.995(3)		1.02(3)		

Table 2. The average sign for various N and n ($\tau = 5$, $\varepsilon = 1$).

N	$n = 1$	2	3	5	7
16	1		0.2221(3)		
32	1		0.0912(5)		
64	1	0.2044(6)	0.0436(4)	0.0120(3)	0.0104(3)
128	1		0.026(1)		

and a right mover. The frequencies of the modes are

$$\omega_\alpha = \sqrt{1 + \frac{4}{\varepsilon^2} \sin^2 \frac{\pi\alpha}{n}} \qquad \alpha = 1, \ldots, A. \tag{27}$$

This leads to a ground-state (vacuum) energy

$$E_0 = \tfrac{1}{2} + \sum_{\alpha=1}^{A} \omega_\alpha \tag{28}$$

and the following energies of one-particle states, numbered by the Fourier mode index α:

$$\Delta E_1(\alpha) = E_1(\alpha) - E_0 = \omega_\alpha \tag{29}$$

where the particle mass is $m = \Delta E_1(0) = 1$.

For $\alpha \ll n$, the equation (29) reproduces the standard formula $\Delta E_1 = \sqrt{m^2 + p^2}$ with the momentum $p = 2\pi\alpha/(\varepsilon n)$.

The mass m can be calculated as the difference between the ground-state energy of the fermionic twin system and that of one individual system. In practice, for finite τ such an estimator also includes contributions from non-zero momentum states. Although they vanish exponentially with τ, for finite τ they may systematically lead to results that are somewhat overestimated[4]. To minimize this unwanted effect one should concentrate the analysis only on the zero-momentum mode $Q = Q_{\alpha=0}$. The effective action density for the zero-momentum mode is given by (5), with q replaced by the zero mode Q.

To determine the energy of Q, we simulate the whole (1+1)-dimensional system, estimate for finite τ the probability that the system is in the zero momentum mode and measure quantities related to Q only. The results are summarized in tables 1 and 2.

Table 1 contains the results for the particle mass. As we can see, the results agree with the theory; in other words, the method works. Unfortunately, the method is limited by the sign problem, which enters the game as a result of the antisymmetrization (19), causing the integrand of (18) to not be positive in general. It forces us to first change the MC weights by taking their absolute value $|\hat{\mathcal{K}}|$ of the integrand in (18), use these modified weights in the

[4] The effect grows with n because the energy separation of momentum modes decreases as n increases. For example, at $\tau = 5$ the maximal effect we measured was of order 10% for $n = 7$.

simulations and then eventually to include the sign of $\hat{\mathcal{K}}$ in the estimators of the measured quantities:

$$\langle \mathcal{O} \rangle = \frac{\langle \mathcal{O} \ \mathrm{sgn}\,(\hat{\mathcal{K}}) \rangle_{|\hat{\mathcal{K}}|}}{\langle \mathrm{sgn}\,(\hat{\mathcal{K}}) \rangle_{|\hat{\mathcal{K}}|}}. \tag{30}$$

The sole exception to this is the quantum system with only one degree of freedom, for which it is possible to show that the sign of the weights is always positive due to cancellations appearing in the two-step transfer matrix.

Generically, one expects the sign problem to create an exponential growth in the computer demands both in n and N, because the computer time required is roughly inversely proportional to the average sign, which typically approaches zero exponentially. To test this, we measured the average sign as a function of n and N. As one can see from table 2, it does indeed decrease with growing N. On the other hand, as can be also seen in the table, for small N the sign is far from zero, but then the results for the particle mass are biased by systematic errors. It is a practical question whether there exists a window in N that has both small enough systematic errors and a large enough average sign. This might be the case for systems which have excited states with relatively large masses that decay over a small number of time slices, such as for instance $SU(3)$ [7].

5. Conclusions

In conclusion, we presented a new method for the determination of excited states in quantum mechanical systems. For quantum mechanics with one degree of freedom, the method allows us to determine recursively the lowest states and their energy. The method can be extended to systems with more degrees of freedom, but in doing so one encounters the sign problem which in many cases can create practical limitations. It may be that applying the recent ideas for defeating the sign problem [8] to the method presented here would lead to an efficient method for field theoretical applications as well.

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