Accurate determination of spectra in discrete-time quantum mechanics

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Various approximation schemes have been proposed which discretize the operator Heisenberg equations of motion. In this paper we demonstrate a simple and accurate method for obtaining the energy spectrum of the theory directly from the discrete-time equations of motion.

Nonlinear operator differential equations of motion cannot be solved in closed form. However, several discretization schemes have been proposed which convert these differential equations to discrete-time operator difference equations which can be solved algebraically.[1-3] In this paper we take the difference scheme proposed in Ref. 1 and show how to obtain directly the energy eigenvalues of the theory.

The procedure we follow is an extension of the ideas discussed in an earlier paper on quantum tunneling.[4] In that paper the continuum Heisenberg equations

$$\dot{q}(t)=p(t),\quad \dot{p}(t)=-V'(q) \tag{1}$$

are replaced by the explicit discrete-time difference equations

$$q_{n+1}=q_n+hp_n-\tfrac{1}{2}h^2V'(q_n)\,, \tag{2a}$$

$$p_{n+1}=p_n-\tfrac{1}{2}h[V'(q_n)+V'(q_{n+1})]\,, \tag{2b}$$

where h is the time-lattice spacing. It had been shown that the lattice scheme in (2) preserves the equal-time commutation relations of the operators q and p.[1]

Because the difference equations (2) are explicit, they can be iterated algebraically to find the operators q_n and p_n after several time steps. However, this procedure is cumbersome. Instead we introduce a set of Fock states and convert to a system of D-dimensional matrix equations. A detailed description of these equations is given in Ref. 4. By iterating these matrix equations using a simple FORTRAN code we can easily obtain q_n and p_n from q_0 and p_0, where n is in the thousands.

The novelty of this paper is that we use the matrix representation for q_n, $n=0,1,2,\ldots,N$, to determine the energy spectrum. To do this we observe that the matrix elements $A_n=\langle 0\,|\,q_n\,|\,1\rangle$ form a numerical time sequence. We compute the discrete Fourier transform of this time sequence:

$$\tilde{A}_m=\frac{1}{N+1}\sum_{n=0}^{N}A_n\exp\left[\frac{2\pi imn}{N+1}\right]. \tag{3}$$

When we plot $|\tilde{A}_m|^2$ vs m we observe sharply peaked spikes. A spike located at $m=m_0$ on the discrete frequency lattice corresponds to a continuum energy of $E_0=2\pi m_0/[(N+1)h]$. In fact, the spikes are so sharply

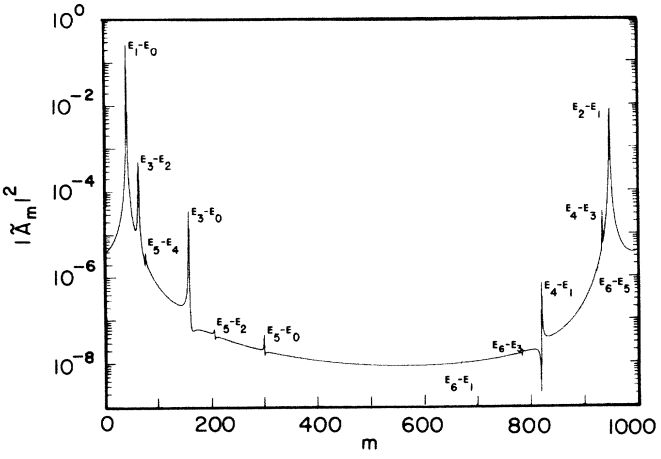

FIG. 1. A semilogarithmic plot of $|\tilde{A}_m|^2$ in (3) vs m for the anharmonic oscillator $V(q)=gq^4$ with $g=0.885$. The spikes give extremely accurate approximations to energy differences E_j-E_k of the exact spectrum. To read off the predicted energy differences, we note that one unit on the horizontal scale corresponds to an energy increment of $\Delta E=2\pi/[(N+1)h]$. Energy differences are measured from both the left axis and the right boundary (see Ref. 5).

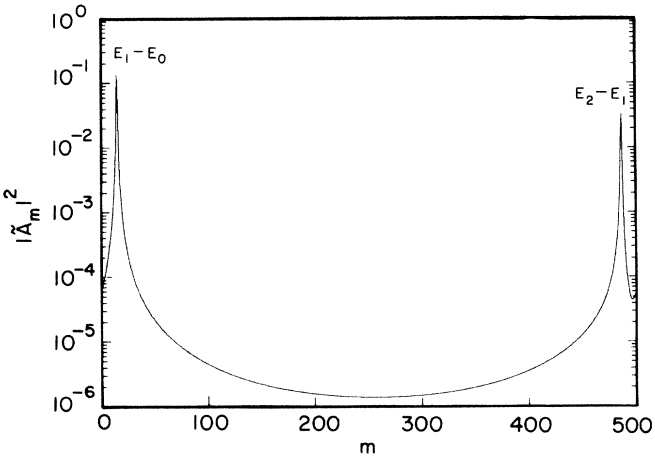

FIG. 2. A semilogarithmic plot of $|\tilde{A}_m|^2$ in (3) vs m for the harmonic oscillator $V(q)=9q^2/2$. The locations of the spikes determine the energies to within 2%. Because the harmonic oscillator is a free theory, only two spikes occur.

TABLE I. Comparison between exact eigenvalue differences for the anharmonic oscillator $V(q)=gq^4$, $g=0.885$, and the approximate eigenvalue differences obtained in the following manner. We find the integer values of m for which $|\tilde{A}(m)|^2$ is a local maximum. The energy difference E_j-E_k is then predicted to be $2\pi m/[(N+1)h]$. This procedure gives relative errors of order 1–3% as shown. However, this procedure can be drastically refined by using nearby values of $|\tilde{A}(m)|^2$ to interpolate the precise (noninteger) value of the location of the maximum.

Energy difference	Exact	Approximate	Relative error (q)
E_1-E_0	1.728	1.674	3.1%
E_2-E_1	2.142	2.218	−3.5%
E_3-E_2	2.537	2.595	−2.3%
E_4-E_3	2.790	2.846	−2.0%
E_5-E_4	3.000	3.097	−3.2%
E_6-E_5	3.210	3.306	−3.0%
E_3-E_0	6.407	6.487	−1.2%
E_4-E_1	7.469	7.659	−2.5%
E_5-E_2	8.327	8.454	−1.5%
E_6-E_3	9.000	9.165	−1.8%
E_5-E_0	12.20	12.39	−1.6%
E_6-E_1	13.68	13.98	−2.2%

peaked that it is necessary to plot $|\tilde{A}_m|^2$ vs m on a semilogarithmic scale.

The accuracy of this procedure increases with increasing N and D. However, for modest values of these parameters we obtain a very accurate representation of the spectrum. For example, with $D=11$ and $N=1000$ we solved the anharmonic oscillator with $V(q)=gq^4$.

In Fig. 1 we graph $|\tilde{A}_m|^2$ for $g=0.885$. Observe that odd-parity versus even-parity energy differences E_j-E_k are measured from the left axis, while even-parity minus odd-parity energy differences are measured from the right boundary.[5]

In Table I we compare the exact values of E_j-E_k with the approximate values obtained with this numerical scheme. The percentage relative error typically ranges from one to three percent.[6]

In Fig. 2 we plot $|\tilde{A}_m|^2$ for the harmonic oscillator $V(q)=9q^2/2$ with $D=11$ and $N=500$. The left spike corresponds to E_1-E_0. The exact value for E_1-E_0 is 3.0 and the predicted value is 2.93, giving a relative error of 2%. The right spike corresponds to E_2-E_1 and the prediction is also correct to 2%.

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[5]To explain the distribution of spikes in Fig. 1 we make the following argument. We compute the matrix element $\langle 0|q(t)|1\rangle$ by inserting complete sets of energy eigenstates $|E_i\rangle$:

$$\langle 0|q(t)|1\rangle=\sum_j\sum_k\langle 0|E_j\rangle\langle E_j|q(t)|E_k\rangle\langle E_k|1\rangle$$
$$=\sum_j\sum_k a_{jk}e^{i(E_j-E_k)t},$$

where $a_{jk}=\langle 0|E_j\rangle\langle E_j|q(0)|E_k\rangle\langle E_k|1\rangle$. Note that $a_{jk}=0$ unless j is even and k is odd. On the lattice $t=nh$ and the discrete Fourier transform in (3) requires that we compute the sum

$$\sum_{n=0}^{N}e^{inh(E_j-E_k)}e^{i2\pi nm/(N+1)}.$$

Clearly, a spike will occur when

$$h(E_j-E_k)+\frac{2\pi m}{N+1}=0,2\pi,\ldots.$$

Thus,

$$E_{\text{odd}}-E_{\text{even}}=\frac{2\pi m}{(N+1)h},$$

which is measured from the left axis, and

$$E_{\text{even}}-E_{\text{odd}}=\frac{2\pi(N+1-m)}{(N+1)h},$$

which is measured from the right boundary.

[6]The procedure used in this paper is clearly suited for use in the Heisenberg picture in Minkowski space. The usual Monte Carlo lattice procedure for finding energy levels consists of determining the exponential decay constants of correlation functions in Euclidean space.