PHYSICAL REVIEW A VOLUME 39, NUMBER 7 APRIL 1, 1989

Quantization of lattice Schrödinger operators via the trigonometric moment problem

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(Received 20 June 1988)

We consider the spectral problem for lattice Schrödinger operators with polynomial potentials. The eigenfunctions in the discrete spectrum of these operators correspond to the *trigonometric moments* of the periodic solutions of certain ordinary differential equations. Relying on this observation, the classical theory of moments permits the derivation of exact analytical and numerical bounds to the eigenvalues.

I. INTRODUCTION

Lattice quantum systems are useful models for a variety of physical phenomena, ranging from phase transitions to subnuclear particles. Among these, one-dimensional lattice Schrödinger operators are particularly important, hence their mathematical properties have been extensively investigated.[1] These operators describe electron conduction in disordered, periodic, or quasiperiodic media.[2–4] They also arise in the quantization of certain classically chaotic dynamical systems, such as the *kicked rotator*.[5,6] In these problems, the spectral properties of these operators are of paramount importance in characterizing the dynamics: they determine, for instance, the electrical conductivity of a medium, or the quasiperiodic versus unlimited evolution of the energy of a kicked rotator.

Since the determination of spectral properties may be nontrivial,[7,8] it is important to develop new analytical methods to analyze this problem. In this paper we introduce a method to compute the discrete spectrum (when present) of lattice Schrödinger operators. This method is analytical, but can be readily adapted to provide computer assisted proofs. Handy and Pei[9] have shown that a direct application of the classical theory of moments can determine upper and lower bounds to the ground-state energy of discretized Schrödinger operators. Nevertheless, their analysis is ineffective in the limit of large lattice spacings. A different formulation based on trigonometric moments[10] is best suited to treat this case, and is here described.

The reformulation of the lattice spectral problem in terms of a periodic differential equations is crucial to our theory. A by-product of this work is an interesting result: one is able to compute the gap edges in the spectrum of the continuous Mathieu equation.[11]

II. LATTICE EIGENFUNCTIONS AND TRIGONOMETRIC MOMENTS

The Schrödinger operators we will consider are of the form,

$$H: D\subset l^2(Z)\rightarrow l^2(Z) ,$$
$$H(e_n)=-\frac{1}{a^2}(e_{n+1}+e_{n-1}-2e_n)+V(an)e_n \qquad (1)$$

where e_n is a canonical basis set for $l^2(Z)$, the space of square summable sequences. If V is a well-behaved potential, H is essentially self-adjoint[12] on a proper domain D in l^2. We will focus on systems with polynomial potentials,

$$V(x)=\alpha_0x^{2p}+\alpha_1x^{2p-1}+\cdots+\alpha_{2p} ,$$
$$\alpha_0>0,\ p \text{ integer} , \qquad (2)$$

with leading even power, characterized by a discrete energy spectrum.

We can expand the general lattice wave function as $\psi=\sum_n \psi_n e_n$, $\psi_n=(e_n,\psi)_{l^2}$, so that the spectral problem can be written in the usual form,

$$(H\psi)_n=-\frac{1}{a^2}(\psi_{n+1}+\psi_{n-1}-2\psi_n)+V(an)\psi_n=E\psi_n . \qquad (3)$$

We see from Eq. (3) that the limit $a\rightarrow\infty$ is singular, as the coefficient in front of the discretized Laplacian vanishes. This singularity was at the origin of the problems encountered in Ref. 9.

Let us now consider the following expression:

$$\phi(k)=\sum_{l=-\infty}^{\infty}\exp(-ikl)\psi_l , \qquad (4)$$

which represents the formal Fourier transform of the lattice wave function ψ_l. If ψ_l is an eigenstate of the Hamiltonian (3) in l^2 the expression (4) has a precise meaning. It is possible to show [e.g., by considering the transfer matrix of Eq. (3)] that the coefficients $|\psi_n|^2$ decay (at least) exponentially at $\pm\infty$ if ψ is an eigenfunction.[13] It then follows that $\phi(k)$ is analytical in a strip along the real axis (possibly extending to the full complex k plane). Also, $\phi(k)$ is periodic with period 2π.

Conversely, if $\phi(k)$ is such a function, the coefficients

$$\psi_n=\frac{1}{2\pi}\int_0^{2\pi}\exp(ink)\phi(k)dk , \qquad (5)$$

are at least exponentially decaying. Using the representation (5), we will then transform the spectral problem (3) into a differential equation for $\phi(k)$. In other words, classical results in the theory of Fourier series establish a one-to-one correspondence between analytical periodic ϕ solutions of a continuous differential equation and l^2 ψ eigenfunctions of the original spectral problem.

Equation (5) is the inversion formula for the Fourier transform. It also shows that ψ_n are the *trigonometric moments* of the measure $d\mu(k)=\phi(k)dk$. Let us assume for the moment that this measure is positive: $d\mu(k)\geq 0$. This is indeed true for the ground state;[12] a generalization to treat the excited states is described in a later section.

In general, for a positive measure $d\mu(k)$, the inequalities

$$\int_0^{2\pi}\left|\sum_m c_m \exp(imk)\right|^2 d\mu(k)\geq 0 \tag{6}$$

hold for any finite set of complex coefficients c_m. They can be transformed into the quadratic form inequalities,

$$\sum_{m,n=0}^{N} c_n^* \psi_{m-n} c_m \geq 0, \quad 0\leq N<\infty \ . \tag{7}$$

It is to be noted that $\psi_m^* = \psi_{-m}$ for real $\phi(k)$; thus the finite matrix ψ_{m-n} in Eq. (7) is Hermitian. According to the classical theory of moments[10] the relations (7) are equivalent to the Toeplitz determinantal inequalities,

$$\Delta_N(\psi_{m-n})=\text{Det}\begin{bmatrix}\psi_0 & \psi_{-1} & \psi_{-2} & \cdots & \psi_{-N}\\ \psi_1 & \psi_0 & \psi_{-1} & \cdots & \psi_{1-N}\\ \vdots & & & & \vdots\\ \psi_N & \psi_{N-1} & \psi_{N-2} & \cdots & \psi_0\end{bmatrix}\geq 0 \ , \tag{8}$$

for $0\leq m,\ n\leq N<\infty$. The infinite set of inequalities (8) is also sufficient to ascertain that a sequence of entries ψ_n be the trigonometric moments of a positive measure.[10]

Equation (3) can be interpreted as a recursion relation for the coefficients ψ_n. By induction, it implies that all ψ_n may be written in the form

$$\psi_n=\sum_{m\in M} c_m^{(n)}(E)\psi_m + d^{(n)}(E) \ , \tag{9}$$

where the coefficients $c_m^{(n)}(E)$ and $d^{(n)}(E)$ can be obtained exactly as a function of $V(x)$. In the language of Ref. 14, the trigonometric moments may be generated as a function of the energy E and a set of *missing moments* ψ_m, $m\in M$. Here, $M=\{1\}$, because the second-order nature of Eq. (3) permits to express all moments as linear combinations of ψ_0, ψ_1, and the former may be eliminated by normalization.

Inserting Eq. (9) in Eq. (8) yields an infinite set of inequalities which constrain E and the missing moments into a convex region. This region rapidly shrinks to a point, as N increases. We now illustrate our method in relation to the lattice harmonic oscillator.

III. LATTICE HARMONIC OSCILLATOR AND MATHIEU EQUATION

Let us determine the ground-state energy E_0 of the discretized harmonic oscillator, defined by Eq. (3) with

$$V(an)=a^2n^2 \ . \tag{10}$$

Using the representation (5), and under the hypothesis of exponentially fast decrease of ψ_n, the spectral problem (3), (10) is equivalent to finding the analytical, 2π periodic solutions of the Mathieu differential equation,

$$-\phi''(k)-[\lambda-2\epsilon\cos(k)]\phi(k)=0 \ , \tag{11}$$

where $\epsilon\equiv -a^{-4}$ and

$$\lambda=E/a^2-2/a^4 \ . \tag{12}$$

Following the standard theory of periodic Schrödinger operators,[15] such solutions $\phi(k)$ are eigenfunctions of $H(\theta)$ for $\theta=0$. According to the notation of Ref. 15,

$$H(\theta)=\left[-\frac{d^2}{dk^2}\right]_\theta + V(k) \ , \tag{13}$$

is an operator on the subspace of $L^2[0,2\pi]$ subject to the boundary conditions,

$$\begin{aligned}\phi(2\pi)&=e^{i\theta}\phi(0) \ ,\\ \phi'(2\pi)&=e^{i\theta}\phi'(0) \ .\end{aligned} \tag{14}$$

$H(\theta)$ has purely discrete spectrum.

We now focus on the ground state of $H(\theta=0)$. It is a real, positive,[12] even $[\phi(k)=\phi(2\pi-k)]$ function. Its trigonometric moments are also real, positive, and even: $\psi_n=\psi_{-n}$. These properties are indeed exceptional; we will show in Sec. IV a first generalization to a wider situation. The moments ψ_n are at the same time the components of the ground state of the original l^2 problem, as seen from Eq. (12). We have so proved that the sequence $(\psi_n)_{n\in N}$ satisfies the inequalities (7) and (8). We are now going to use this fact.

The next step in our theory comes after noticing that, if we choose the (arbitrary) normalization $\psi_0=1$, the ψ_n may be recursively generated as functions of the energy from Eqs. (3) and (10),

$$\begin{aligned}\psi_0&=1 \ ,\\ \psi_1&=(2-a^2E_0)/2 \ ,\\ \psi_2&=\psi_1(2\psi_1+a^4)-1 \ ,\end{aligned} \tag{15}$$

etc. We notice that in this case we do not have missing moments in Eq. (9). The $\Delta_{N=1}$ constraint, together with the positivity of ψ_1 implies that $0<E_0<2/a^2$. The $\Delta_{N=2}$ constraint, plus $\psi_1>0$ provides the following bounds (valid for $a>\sqrt{2}$, after majorization of a square root),

$$2/a^2-4/a^6<E_0<2/a^2 \ . \tag{16}$$

They are to be compared to the bounds derived in Ref. 9,

$$\frac{2}{a^2}-\frac{20}{a^6}<\tfrac{1}{10}[-a^2+(a^4+40)^{1/2}] < E_0 < \tfrac{1}{8}[a^2+(a^4+112)^{1/2}] \ . \tag{17}$$

In the limit of large a the bounds (16) are tight while only the lower bound in Eq. (17) is significant. It is noteworthy that a second-order, perturbative analysis (obtained by treating the kinetic energy as a perturbation) yields the result

$$E_0 \simeq 2/a^2 - 1/(2a^6) , \quad (18)$$

which is in agreement with Eq. (16).

In Table I we quote the numerical energy bounds obtained for various values of a and N. Accurate results can be obtained using very low-order determinant inequalities. Figure 1 draws the ground state and the next two symmetric excited states (to be discussed in Sec. IV). We notice that the ground-state lattice eigenfunction is exponentially localized in a very narrow region. This is the effect of the singular character of the problem for large lattice spacings a. In this limit, in fact, the kinetic energy becomes a perturbation of $V(x)$, which is diagonal over the canonical basis of l^2.

IV. EXCITED STATES OF THE HARMONIC OSCILLATOR AND THE SPECTRUM OF THE MATHIEU EQUATION

We now turn our attention to the excited states of the Hamiltonian (3) and (10). We have shown their one-to-one correspondence to the eigenfunctions of $H(0)$, Eq. (13). These latter eigenfunctions do not possess a definite signature and the previous approach must be generalized. Thanks to their continuity properties, we can nonetheless say that for each $\phi(k)$ there exists a constant c such that

$$f_c(k) = \phi(k) + c > 0 . \quad (19)$$

We now denote by $\chi_n(c)$ the trigonometric moments of $f_c(k)$. They are related to the moments of $\phi(k)$ in a very simple manner,

$$\chi_n(c) = \psi_n + c\delta_{n,0} . \quad (20)$$

We can now apply the theory of Sec. III to the sequence $(\chi_n)_{n\in N}$. In the case of symmetric states, this sequence is simply obtained by Eqs. (15) and (20). The case of antisymmetric solutions can be dealt with in a similar manner. The inequalities (8) $\{\Delta_N[\chi_{m-n}(c)] \ge 0\}$ can now be imposed, together with the condition $0 \le c \le C_+$, where C_+ is chosen arbitrarily large. As a result, the inequalities constrain E and c to a set of connected "feasibility" regions in the E-c space, one for each eigenvalue, which can be numerically determined through the techniques of linear programming.[14,16]

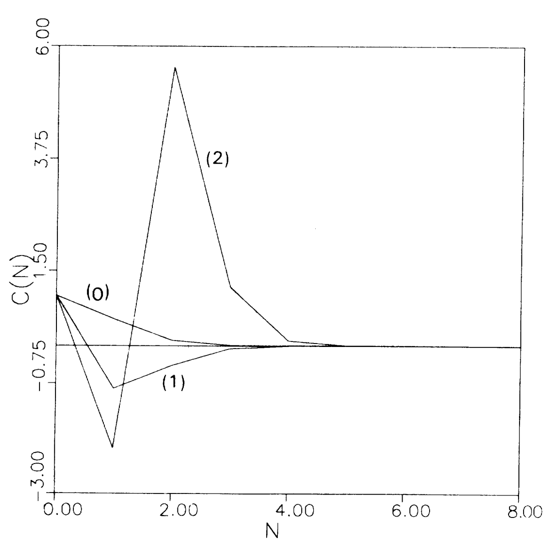

FIG. 1. Lattice configuration $c(N) = \psi_N$ of the ground state (0) and the first two symmetric excited states (1,2) of the harmonic Hamiltonian (10). Due to the symmetry, only positive N have been reported. The lines between points are merely to guide the eye. The normalization $c(0) = 1$ has been chosen.

TABLE I. Bounds for the ground-state energy of the discretized harmonic oscillator. The inequalities $\psi_n \ge 0$ and $\Delta_N(\psi_{j-k}) \ge 0$, for $n, N \le \bar{N}$ have been used.

a	$\bar{N}$	$E_0^{(-)}$	$E_0^{(+)}$
1	2	0.43	1.01
1	4	0.919	0.930
1	6	0.929 849	0.929 871
1	8	0.929 870 284	0.929 870 296
2	2	0.43	0.47
2	3	0.4684	0.4690
2	4	0.468 95	0.468 97
2	5	0.468 960 5	0.468 960 7
5	2	0.079 744	0.079 873
5	3	0.079 871 94	0.079 872 01

The "completeness" of the energy spectrum computed by the above procedure can be numerically checked by gradually increasing the value of C_+. This creates new feasibility regions, other than the one previously computed, corresponding to newly determined eigenvalues. If these are greater than the previous values, we are assured that the sequence of levels computed is complete up to the highest determined eigenstate.

In Table II we report the bounds related to the first three even excited states of the harmonic oscillator, as a function of the order of inequalities employed. The results are very accurate. To estimate the performance of the method for higher excited states, we tabulated in Table III the data for the first six even excited states, obtained at fixed $\bar{N}$. While the absolute precision gets worse by increasing the energy, the relative error diminishes, at

TABLE II. Energy bounds for the three lowest symmetric states of the discretized ($a=1$) harmonic oscillator. The upper estimate C_+ is 10^3.

$\bar{N}$	j	$E_j^{(-)}$	$E_j^{(+)}$
6	0	0.90	0.97
	1	3.59	3.84
	2	6.02	6.29
7	0	0.929	0.931
	1	3.703	3.711
	2	6.158	6.167
8	0	0.929 85	0.929 89
	1	3.707 19	3.707 35
	2	6.162 36	6.162 55

TABLE III. Energy bounds for the six lowest symmetric states of the discretized ($a=1$) harmonic oscillator. The number of moments used, $\bar{N}=8$ is kept constant. Δ is the absolute error (difference of the upper and lower bounds) while δ is the corresponding relative precision in the determination of the eigenenergy.

j	$E_j^{(-)}$	$E_j^{(+)}$	Δ_j	δ_j
0	0.929 85	0.929 89	4×10^{-5}	4.3×10^{-5}
1	3.707 19	3.707 35	1.6×10^{-4}	4.3×10^{-5}
2	6.162 36	6.162 55	1.9×10^{-4}	3.0×10^{-5}
3	11.057 34	11.057 60	2.6×10^{-4}	2.4×10^{-5}
4	18.031 66	18.032 02	3.6×10^{-4}	2.0×10^{-5}
5	27.019 97	27.020 45	4.8×10^{-4}	1.8×10^{-5}

least in the scale covered by our computations.

It is evident from the one-to-one correspondence between $H(0)$ and the lattice problem that the theory developed here immediately provides *half* of the gaps and of the bands of the spectrum of the periodic Mathieu equation. Yet, the same formalism can be applied to $H(\pi)$, the operator with antiperiodic boundary conditions, as defined by Eq. (14): a different lattice operator is now associated with $H(\pi)$—a shifted quadratic harmonic oscillator. As a consequence, the spectrum of the Mathieu equation can be exactly determined through our method.

V. THE SEXTIC ANHARMONIC OSCILLATOR

A different example is represented by the sextic anharmonic oscillator,

$$V(an)=a^2n^2+a^6n^6 \ . \tag{21}$$

This potential leads to a differential equation of sixth order for $\phi(k)$,

$$\frac{d^2\phi}{dk^2}(k)+a^4\frac{d^6\phi}{dk^6}(k)+[\lambda+2\epsilon\cos(k)]\phi(k)=0 \ . \tag{22}$$

In the above, λ and ϵ are still given by Eq. (12). This is no longer a Schrödinger equation. The preceding analysis can nevertheless be applied, yielding the results summarized in Table IV, for the ground and first symmetric excited states.

TABLE IV. First two lowest-lying symmetric states for the discretized ($a=1$) sextic anharmonic oscillator. The upper estimate C_+ is varied to show the corresponding sensitivity of the bounds.

$\bar{N}$	C_+	j	$E_j^{(-)}$	$E_j^{(+)}$
4	10^3	0	1.26	1.28
	10^3	1	4.71	4.73
5	10^3	0	1.264 861 6	1.264 867 3
	10^3	1	4.719 977	4.719 983
	10^4	0	1.264 84	1.264 89
	10^4	1	4.7199	4.7201
6	10^3	0	1.264 864 442 0	1.264 864 442 4
	10^3	1	4.719 980 458 1	4.719 980 458 6
	10^5	0	1.264 864 42	1.264 864 45
	10^5	1	4.719 980 3	4.719 980 6

VI. CONCLUSIONS

We have developed an exact trigonometric moment problem quantization for lattice Schrödinger operators. By implementing the Hankel-Hadamard inequalities of the classical theory of moments, we have derived analytical and numerical bounds to the eigenvalues of the lattice harmonic and sextic anharmonic Schrödinger operators.

This theory can also provide information on certain periodic differential operators associated by Fourier transformation to the original lattice problem, such as the Mathieu equation corresponding to the lattice harmonic oscillator. Finally, the extension to the multidimensional case is immediate, based on the formalism of Ref. 14.

ACKNOWLEDGMENTS

This research was supported by the National Science Foundation (NSF) under Grant No. RII-8604334. One of us (C.R.H.) was also supported by NSF Grant No. RII-8312. The numerical computations which corroborate this work have been funded by a grant from the Pittsburgh Supercomputing Center.

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