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One-dimensional action billiards and eigenvalues of truncated Hamiltonians

M.A.M. de Aguiar
Departamento de Física do Estado Sólido e Ciência dos Materiais, Instituto de Física "Gleb Wataghin", Universidade Estadual de Campinas, 13081 Campinas, SP, Brazil

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The eigenvalues of a simple one-dimensional Hamiltonian matrix are studied in the framework of "action billiards". We show that the effect of truncating the quantum matrix can be understood in terms of the underlying truncated classical dynamics. The exact spectrum is compared to that of the truncated matrix and the WKB approximation for the billiard. The point where the different calculations start to deviate from one another corresponds to the energy of the first orbit hitting the billiard boundary. Above this energy the truncated spectrum shows quasi-degeneracies, not present in the exact spectrum, due to quantum tunneling between disjoint parts of the classical orbits.

The energy levels of bound systems are the eigenvalues of their corresponding Hamiltonian matrices, which are generally infinite. Since numerical calculations are restricted to finite computer memory, the process of obtaining the eigenenergies consists of diagonalizing a truncated matrix followed by a convergence test. In several situations, like in the study of the semiclassical limit of chaotic systems, one is often interested in statistical properties of the spectrum and, therefore, it is essential to have a large number of "converged" energy levels. This might be a very cumbersome job depending on the Hamiltonian system. In a recent paper [1] it was proposed that this difficulty could be overcome by a redefinition of the classical and quantum problems. According to ref. [1], if the original matrix is written in a harmonic oscillator basis, then a new quantum system is defined simply as the finite matrix corresponding to a given truncation of the original matrix. The classical analogue of such a system would be an "action billiard". This is the original classical problem truncated in the action variable. It has been shown in ref. [1] that the properties of action billiards are exactly those of common billiards with only two differences: first, the particle is not free in the accessible region and, second, the phase space is finite. For these systems the quantum diagonalization is always exact and, as far as the semiclassical limit is concerned, they are very good models for numerical studies.

In this Letter we consider a model one-dimensional action billiard but we adopt a slightly different point of view. Here, instead of concentrating on the quantum billiard, we study how the eigenvalues of the truncated matrix depart from the exact calculations, in terms of the truncated classical dynamics. In other words, we explore the connection between quantum basis states and classical orbits for truncated (classical and quantum) systems. This relation has been studied along the years in several different contexts, starting with the WKB method [2]. An important approach, introduced by Wigner [3,4], consists in associating to the wave functions a convenient phase space distribution satisfying a number of desired properties. The semiclassical limit of the Wigner functions associated with the eigenstates was studied in detail by Berry [5,6] and Voros [7,8]. In particular, it has been shown that for integrable systems they tend to concentrate sharply on the classical tori with quantized actions, showing clearly the link between eigenstates and phase space invariant structures (these are simple trajectories for one-

dimensional systems). Finally, wave-packet methods were extensively explored by Heller [9–11], Davies [12–14] and more recently by Littlejohn [15], where classical orbits were used to construct improved basis states adapted to each particular problem. In this paper we study a new aspect of this classical to quantum connection and show that the classical trajectories can be of value to understand the whole spectrum of truncated matrices provided the classical dynamics is itself truncated. As a by-product we derive a reliable criterion for the convergence of the eigenvalues and obtain new insight into the semiclassical behavior of action billiards.

Consider the following Hamiltonian,

$$H(I,\theta)=I+\alpha I\cos^2\theta\,, \tag{1}$$

where (I, θ) are the action and angles variables. The associated quantum operator is

$$\hat{H}=\beta\hbar(ha^+a+\tfrac{1}{2})+\tfrac{1}{4}\alpha\hbar^2(a^2+a^{+2})\,, \tag{2}$$

where a^+, a are the usual creation and annihilation operators for the harmonic oscillator $H=I$ and

$$\beta=1+\tfrac{1}{2}\alpha\,. \tag{3}$$

For non-zero α the phase curves of eq. (1) are not straight lines, and the classical solutions are the level curves

$$I_E(\theta)=\frac{E}{1+\alpha\cos^2\theta} \tag{4}$$

as displayed in fig. 1a. From the quantum point of view α introduces off-diagonal matrix elements. Before considering the corresponding action billiard we notice that the Schrödinger equation for the Hamiltonian (2) can be exactly solved. Indeed, the canonical transformation $(I, \theta)\rightarrow(J, \varphi)$ given by

$$J=\frac{I}{\Omega}\,(\sin^2\theta+\Omega^2\cos^2\theta)\,,$$

$$\operatorname{tg}\varphi=\frac{1}{\Omega}\operatorname{tg}\theta\,, \tag{5}$$

where

$$\Omega=\sqrt{1+\alpha}\,,$$

takes eq. (1) into

$$H(J,\varphi)=\Omega J \tag{6}$$

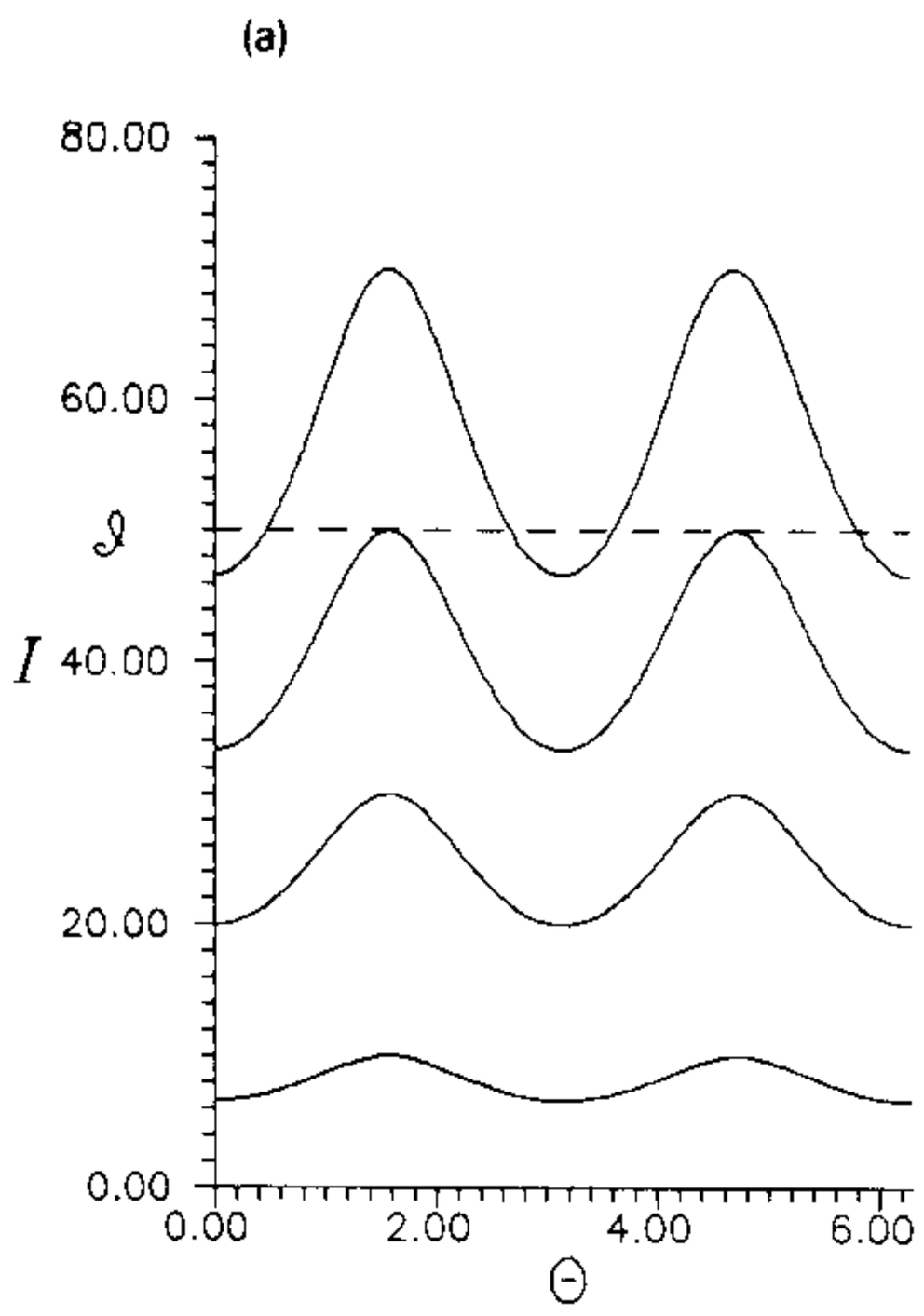


Fig. 1. Level curves for $\alpha=0.5$ in terms of (a) I versus θ and (b) J versus φ. The boundary at $I=\mathscr{L}$ is represented by the dotted line. The pieces of orbits above the boundary are discarded in the action billiard and the segments below the boundary are connected by jumps parallel to the $I=\mathscr{L}$ line.

and maps the level curves (4) into straight lines

$$J_E(\varphi)=\frac{E}{\Omega}$$

as shown in fig. 1b.

The transformed Hamiltonian (6) quantizes as

$$\hat{H}=\Omega\hbar(\hbar b^{+}b+\tfrac{1}{2})$$

and, therefore, the exact eigenenergies are just

$$E_n^{\mathrm{e}}=\hbar\Omega(n+\tfrac{1}{2})\,, \tag{7}$$

where the superscript e stands for "exact".

In the original basis, however, $\hat{H}$ has off-diagonal elements and a truncation will introduce errors in the calculations. Therefore, let us forget for a moment that the exact solution (7) is possible and diagonalize a truncated version of $\hat{H}$ in the basis $|n\rangle$ of $a^{+}a$ with n from 0 to $N-1$. This introduces a classical cut-off at $I=N\hbar\equiv\mathscr{L}$ and the corresponding action billiard is

$$\begin{aligned} H_{\mathrm{b}}(I,\theta,\mathscr{L})&=H(I,\theta), \quad \text{if } I\leqslant\mathscr{L},\\ &=0, \qquad\quad \text{if } I>\mathscr{L}. \end{aligned} \tag{8}$$

The orbits of H_{b} are of two kinds: for energies such that $I(\theta)<\mathscr{L}$ for all θ, they coincide with the corresponding (same energy) orbits of H. For higher energies the orbits of H_{b} consist of the pieces of the corresponding orbits of H where $I<\mathscr{L}$ connected by instantaneous jumps in the angle variable (see ref. [1] for more details).

Notice that the straight line $I=\mathscr{L}$ is mapped into

$$J(\varphi)=\frac{\Omega\mathscr{L}}{1+\alpha\sin^2\varphi} \tag{9}$$

by the transformation (5). The billiard in the variables (J,φ) is also well defined, but has a curved boundary (the inverse transformation $(J,\varphi)\to(I,\theta)$ may be seen as a simple example of how to treat complicate boundaries in more dimensions – see ref. [1]).

The eigenenergies for the action billiard are obtained numerically and we call them E_n^{b}. Plots of E_n versus n are displayed in figs. 2 and 3 for some values of N and α with fixed $\hbar$. From these plots it is clear that E_n^{b} are excellent approximations for E_n^{e} up to a critical energy E^{*}. This corresponds exactly to

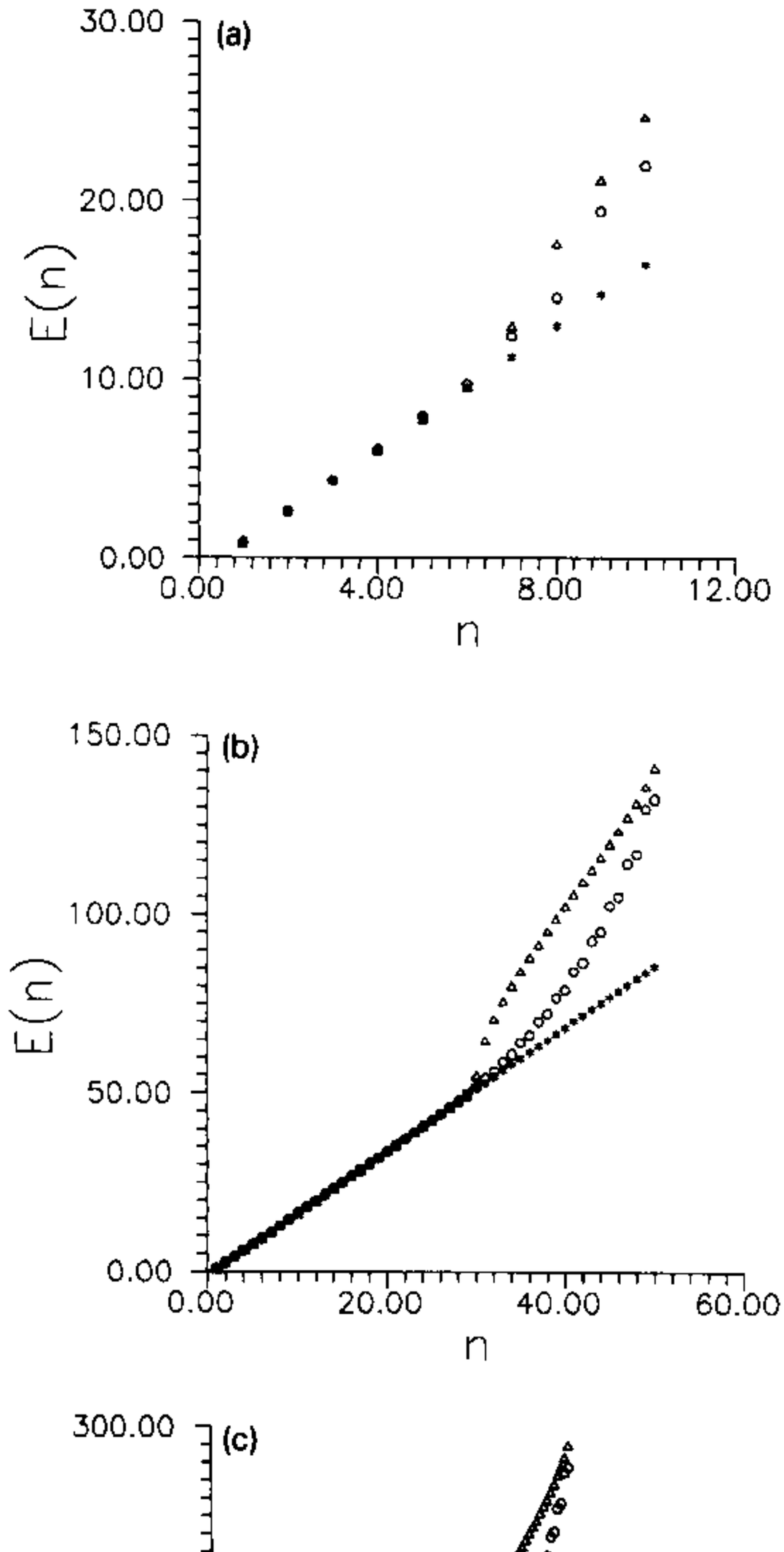
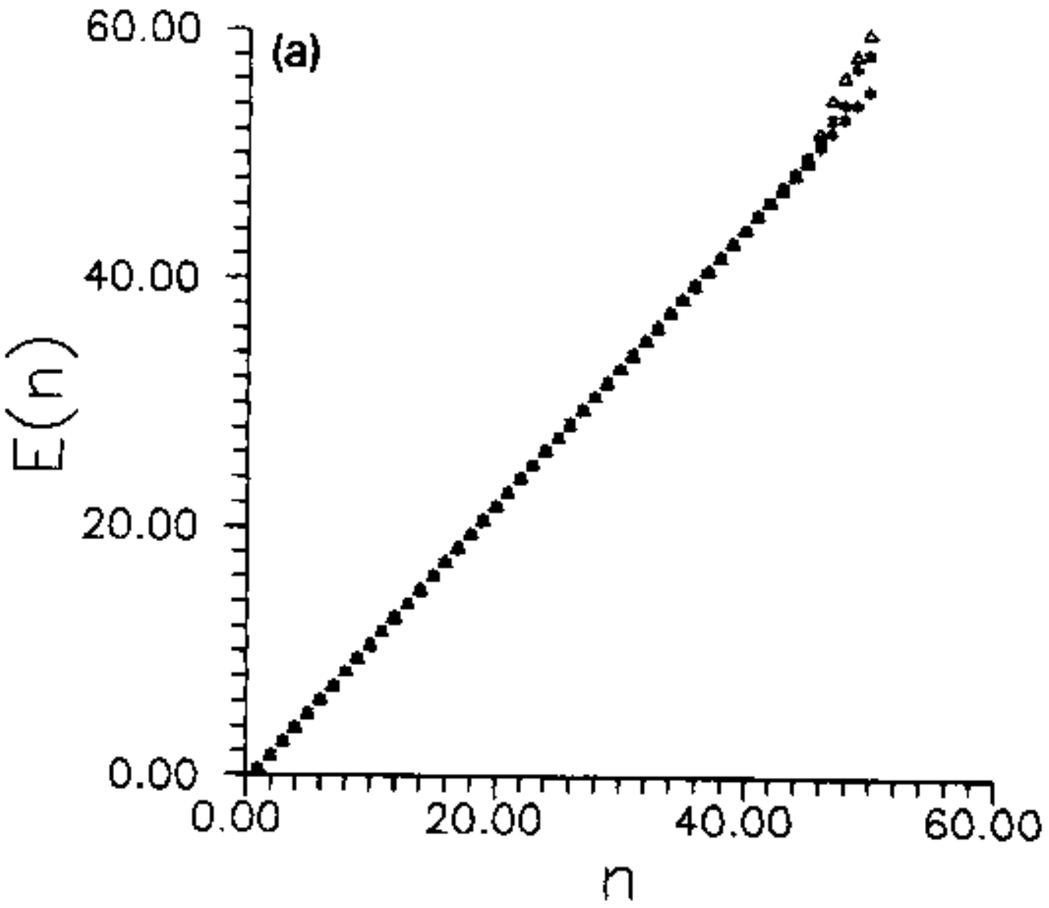
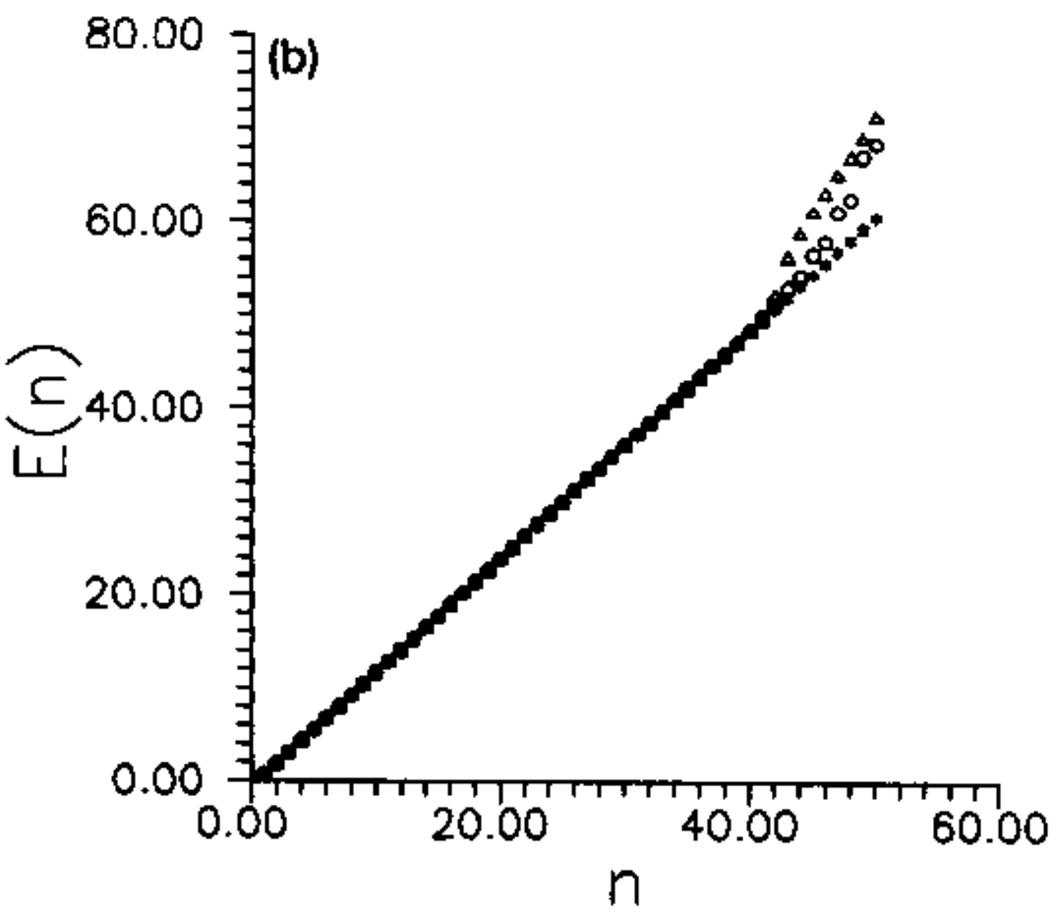


Fig. 2. E_n versus n for $\hbar=1$ and $\alpha=2$. (*) Exact, (○) truncated and (△) WKB results. (a) $N=10$, (b) $N=50$, (c) $N=100$.





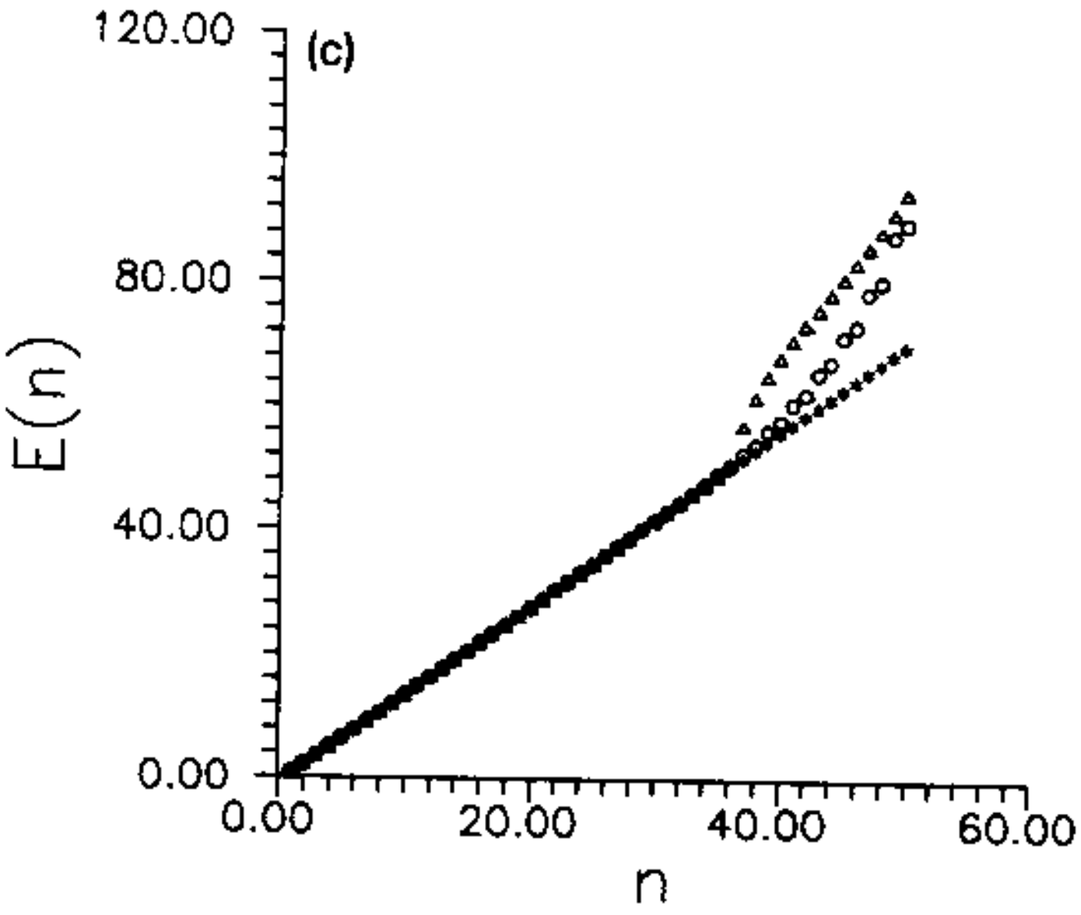


Fig. 3. The same as fig. 2 for $\hbar=1$ and $N=50$. (a) $\alpha=0.25$, (b) $\alpha=0.5$, (c) $\alpha=1.0$.

the energy of the first classical orbit that hits the boundary, $E^*=\mathscr{L}$! From E^* on, $E_n^{\mathrm{b}}>E_n^{\mathrm{e}}$, which is also easy to understand: in terms of action, energy levels are, on average, spaced by $2\pi\hbar$. Since the cut-off at $I=\mathscr{L}$ throws away the area above the boundary in the (I,θ) plane, we have to go higher in energy to overcome the lost area. This argument suggests that the WKB approximation applied to the billiard would give good results. Indeed, for energies below $\mathscr{L}$ no orbit hits the boundary and WKB reads

$$\int_0^{2\pi} I\,\mathrm{d}\theta=\int_0^{2\pi} J\,\mathrm{d}\varphi=(n+\tfrac{1}{2})h\,,$$

or

$$E_n^{\mathrm{WKB}}=\hbar\Omega(n+\tfrac{1}{2})=E_n^{\mathrm{e}},\quad \text{if } E_n^{\mathrm{WKB}}<\mathscr{L}\,. \tag{10}$$

For $E\geqslant\mathscr{L}$ the cut-off introduces a new effect. Since the wave functions must go to zero at the boundary, this corresponds to a particle confined by infinite walls, like a particle in a box. In these situations the WKB approximation reads [2]

$$S\equiv\int_0^{2\pi} I\,\mathrm{d}\theta=nh\,.$$

The integral on the left-hand side is just

$$S=\frac{2\pi E}{\Omega}+\mathscr{L}(2\pi-\theta^*)-\frac{4E}{\Omega}\,\mathrm{tg}^{-1}(\Omega\,\mathrm{cotg}\,\theta^*)\,,$$

where θ^* is the solution of

$$\mathscr{L}=\frac{E}{1+\alpha\cos^2\theta^*}\,\mathrm{mod}(\tfrac{1}{2}\pi)\,.$$

The WKB results are also displayed in figs. 2 and 3 and, indeed they are fairly good approximations for E_n^{b}.

Another interesting feature of the truncated eigenvalues is the neat appearance of doublets for energies close to the boundary. This is probably due to quantum tunneling between the two disjoint parts of the classical truncated orbits.

We conclude that the errors introduced by truncating quantum matrices can be completely understood in terms of a classically truncated system. The results obtained in this way will be in good agreement with the exact eigenvalues for energies corresponding to orbits that never touch the billiard

boundary. This can be used as a convergence criterion for the energy levels, instead of the usual procedures of increasing the matrix size or estimating bounds via variational techniques. For a simple harmonic oscillator and a straigh cut-off, no orbits ever hit the boundary and any truncation will give the exact quantum energies. For a potential like $V(x)=\frac{1}{2}x^2+\lambda x^4$, on the other hand, the classical orbits will be very steep for high energies and no agreement can be expected [16].

From the point of view of action billiards, where the finite diagonalizations are considered exact, we see that the WKB method can still be applied successfully. Moreover, the example considered here shows that the discontinuity of the classical orbits at high energies introduces quasi-degenerate doublets through quantum tunneling, an effect due only to the truncation.

As a last comment we notice that, contrary to Heller's work [10,11], the classical orbits are not being used here to set up new basis states and improve the numerical convergence, but as a guide to understand the quantum behavior of truncated matrices.

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