Energy levels for a square well containing δ-function barriers on a Cantor set

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Energy levels are investigated within a square well containing δ-function barriers on a Cantor set. Particular attention is drawn to the dependence on the strength λ of the δ functions. It turns out that multiple avoided level crossings occur for $\lambda>0$ connecting the limiting cases at $\lambda=0$ and $\lambda=\infty$, which are amenable analytically. The intermediate range is investigated numerically by two different methods: matrix diagonalization and implementation of a boundary condition for the wave function.

The connection of quantum fluctuations, quantum chaos, avoided level crossing, and exceptional points[1] of the underlying Hamiltonian has been the subject of increasing interest recently in the literature.[2–7] It appears that features which are attributed to quantum chaotic behavior prevail, in particular in translational regions from one ordered situation to another.[8,9] Fluctuations in transitional regions are usually associated with quantum-mechanical many-body systems,[10] but they also occur in single-particle problems.[11] In this paper we present results of a model study of a single-particle problem which is born out from mathematically similar situations in quantum-mechanical many-body systems.[8]

We consider a one-dimensional bound-state problem in a square well, which contains δ functions within the square well on a Cantor set. Specifically, let C be the ternary Cantor set which is constructed as follows. Define the open interval

$$I_{n,t}=\left(\frac{3t-2}{3^n},\frac{3t-1}{3^n}\right)$$

and put

$$G_n=\bigcup_{t=1}^{3^{n-1}} I_{n,t},\quad G=\bigcup_{n=1}^{\infty} G_n\ .$$

The set $C=[0,1]\setminus G$ is called the ternary Cantor set. It has cardinal c, is perfect, nowhere dense, and has Lebesgue measure zero. The Hausdorff dimension and capacity of C assume the same value $\ln 2/\ln 3$. The potential for which the bound states are investigated is then defined by

$$V(x)=\begin{cases}\lambda\delta(x) & \text{if } x\in C\\ 0 & \text{if } x\in(0,1)\setminus C\\ \infty & \text{otherwise .}\end{cases}\tag{1}$$

It appears that a Cantor set is an obvious mathematical device which allows infinitely many δ functions within a finite interval while preserving finite lengths of intervals between the δ functions. As we see below these two conditions are crucial to obtain physically interesting patterns. We mention that the Cantor set yields a fractal structure in the partitioning of the unit interval.

The field of "quantum chaos" consists of investigation of quantal systems that are chaotic in the classical limit. The classical limit of our system is completely regular. Indeed, the particle is classically bound between two δ-function barriers (depending on the initial conditions), and the motion is fully periodic, independent of the λ value (except $\lambda=0$). Although the system looks one dimensional, it has properties of multidimensional systems, such as the avoided-crossing phenomena of energy levels, which is well-known in multidimensional-nonintegrable systems. Although there is no classical analog of our model which behaves chaotically we find for the quantized version a behavior which is typically for quantum systems which have a classical analog with chaotic behavior.

Of interest is the spectrum of the Schrödinger equation as a function of the strength λ of the δ functions. Since our interest is concerned with avoided level crossings we have to reduce the problem to existing internal symmetries to obtain eventually an irreducible spectrum. The only symmetry in question here is parity, and we focus our attention on even-parity solutions, where the wave function is symmetric with respect to the point at $x=0.5$.

The positive-parity spectrum is known at the two limiting points $\lambda=0$ and $\lambda=\infty$. For $\lambda=0$ we find

$$k_n/\pi=(2n+1),\quad n=0,1,\ldots\tag{2}$$

(we prefer to use $k_n=\sqrt{E_n}$, where E_n denotes the energy spectrum). For the latter limit ($\lambda=\infty$) we have an infinite superposition of harmonic sequences originating from the eigenvalues relating to the finite intervals between the δ functions. We find

$$k_n^{(1)}/\pi=3(2n+1)\ \text{ from the interval }\left[\tfrac{1}{3},\tfrac{2}{3}\right],$$

$$k_n^{(2)}/\pi=9(n+1)\ \text{ from }\left[\tfrac{1}{9},\tfrac{2}{9}\right]\text{ and }\left[\tfrac{7}{9},\tfrac{8}{9}\right],$$

$$k_n^{(3)}/\pi=27(n+1)\ \text{ from }\left[\tfrac{1}{27},\tfrac{2}{27}\right],\ldots,\left[\tfrac{25}{27},\tfrac{26}{27}\right],$$

sequence is twofold degenerate ,

$$\cdots\tag{3}$$

$$k_n^{(s)}/\pi = 3^s(n+1) \quad \text{from} \left[\frac{1}{3^s},\frac{2}{3^s}\right],\ldots,\left[\frac{3^s-2}{3^s},\frac{3^s-1}{3^s}\right],$$

sequence is $2^{(s-2)}$-fold degenerate ,

$\ldots$,

where $n=0,1,\ldots$. Obviously, both limiting cases give rise to order as expressed by the harmonic spectra. As the two regimes are of a very different nature, the transition from the one to the other is of particular interest.

Two methods are at our disposal to explore the intermediate regime. The one is to solve the Schrödinger equation directly, the other is based on a matrix representation of H and its diagonalization. The second method seems to be more interesting for theoretical reasons, while the first method serves as an independent numerical test. For convenience we shift in the following the whole interval [0,1] to the left by $\frac{1}{2}$. Denoting the general solution in the ith interval by $A_i\cos kx + B_i\sin kx$, we have, up to a common factor, which is of no interest, for $x\in[-\frac{1}{6},\frac{1}{6}]$ the values $A_1=1$ and $B_1=0$. The coefficients A_i and B_i in the adjacent intervals are found from the requirement that the wave function be continuous and its derivative have a jump $\lambda\psi(x_i)$. This establishes a linear relationship between the coefficients in adjacent intervals. In this way we obtain for the interval next to $[-\frac{1}{6},\frac{1}{6}]$,

$$\begin{bmatrix} A_2 \\ B_2 \end{bmatrix} = \begin{bmatrix} 1-(\lambda/2k)\sin 2kx_2 & -(\lambda/2k)(1-\cos 2kx_2) \\ (\lambda/2k)(1+\cos 2kx_2) & 1+(\lambda/2k)\sin 2kx_2 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \tag{4}$$

and for all further intervals

$$\begin{bmatrix} A_i \\ B_i \end{bmatrix} = \prod_{j=2}^{i} \begin{bmatrix} 1-(\lambda/2k)\sin 2kx_j & -(\lambda/2k)(1-\cos 2kx_j) \\ (\lambda/2k)(1+\cos 2kx_j) & 1+(\lambda/2k)\sin 2kx_j \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \tag{5}$$

where the matrix product runs over the strictly ordered Cantor set in one direction, since the individual matrices do not commute. Recall that, for symmetry reasons, we may choose $x_j>0$, i.e., the product runs from $x_2=\frac{1}{6}$ towards $x_\infty=\frac{1}{2}$. The spectrum is obtained from the boundary condition

$$A_\infty\cos\frac{k}{2}+B_\infty\sin\frac{k}{2}=0\ , \tag{6}$$

ensuring that the wave function vanishes at the boundary of the square well, i.e., $x_\infty=\frac{1}{2}$. We address the question of the convergence of the product in Eq. (5) as well as its numerical implementation below.

To obtain a matrix representation of the underlying Hamiltonian we choose as a basis in $L^2[-\frac{1}{2},\frac{1}{2}]$, the complete set of the symmetric wave functions of the unperturbed ($\lambda=0$) problem, i.e., $\sqrt{2}\cos(m\pi x)$, with m odd. The interacting part, viz.,

$$\langle n|H_{\rm int}|m\rangle = 2\lambda\sum_{\{j\}}\cos(n\pi x_j)\cos(m\pi x_j)\ , \tag{7}$$

where the sum runs over all points of the Cantor set, can be rewritten into terms of the form $\sum_j\exp(\pm i\pi q x_j)$ with $q=n+m$ and $q=n-m$. While these sums contain 2^s-2 terms in the sth generation of the partitioning of the interval $[-\frac{1}{2},\frac{1}{2}]$, it can be shown that

$$\sum_{\{j\}>0}\exp(i\pi q x_j)=\exp\frac{i\pi q}{6}\left[\prod_{r=2}^{s}\left[1+\exp\frac{2i\pi q}{3^r}\right]+\sum_{v=0}^{s-2}\prod_{r=2}^{s-v-1}\left[1+\exp\frac{2i\pi q}{3^r}\right]\exp\frac{i\pi q}{3^{s-v}}\right], \tag{8}$$

where the sum is extended only over the positive points of the Cantor set. To obtain this result the ternary representation of the Cantor set is helpful. The advantage of the right-hand side is twofold: (i) a sum of 2^s terms has been reduced to products of s terms and (ii) the rather amazing n and m dependence of $\langle n|H_{\rm int}|m\rangle$ can be understood.

As they stand, the products in Eqs. (5) and (8) diverge when $s\to\infty$. This is related to the fact that the strength λ must tend to zero accordingly. From Eq. (8) it is obvious that $\lambda=G2^{-s}$ is required, where G is an effective strength. Denoting the right-hand side of Eq. (8) by $Z_s(q)$ we therefore obtain

$$\langle n|H_{\rm int}|m\rangle = \lim_{s\to\infty} G2^{-s}{\rm Re}[Z_s(n+m)+Z_s(n-m)]\ . \tag{9}$$

The full Hamiltonian matrix to be diagonalized is therefore

$$H_{n,m}=n^2\pi^2\delta_{n,m}+\langle n|H_{\rm int}|m\rangle,\quad n=1,3,5,\ldots\ . \tag{10}$$

The numerical calculation of the matrix elements is efficiently achieved using Eq. (8), as for any fixed n and m the products in Eq. (8) converge fast. The actual values of the matrix elements seem to be rather erratic. In Fig. 1 we illustrate the diagonal elements of $\langle n|H_{\rm int}|m\rangle$ with n running from 1 to 2400. We stress, however, that the diagram would look qualitatively similar had we chosen any other side-diagonal or row or column. The pattern can in principle be understood from Eq. (8): for large values of m and n, $Z_\infty(n\pm m)$ is generically small, since the argument of the exponential, i.e., $2i(n\pm m)\pi/3^r$ closely approaches an odd integer times $i\pi$ for some of r,

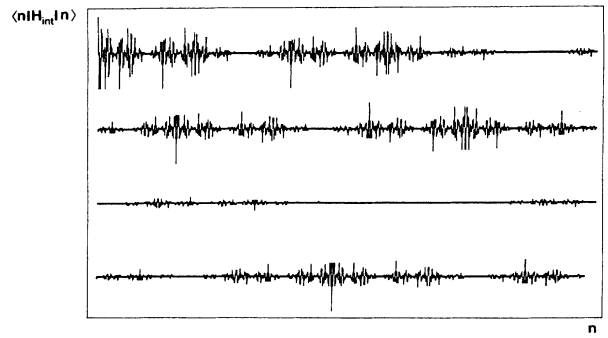

FIG. 1. The first 2400 diagonal elements of $\langle n|H_{\rm int}|m\rangle - 1$. The first row shows the elements up to 600, the second row up to 1200, etc. The center line of each row indicates the zero line, the maximal values above (minimal values below) correspond to value unity (minus unity). Note that the matrix elements are never strictly zero, they only appear so by the scale chosen.

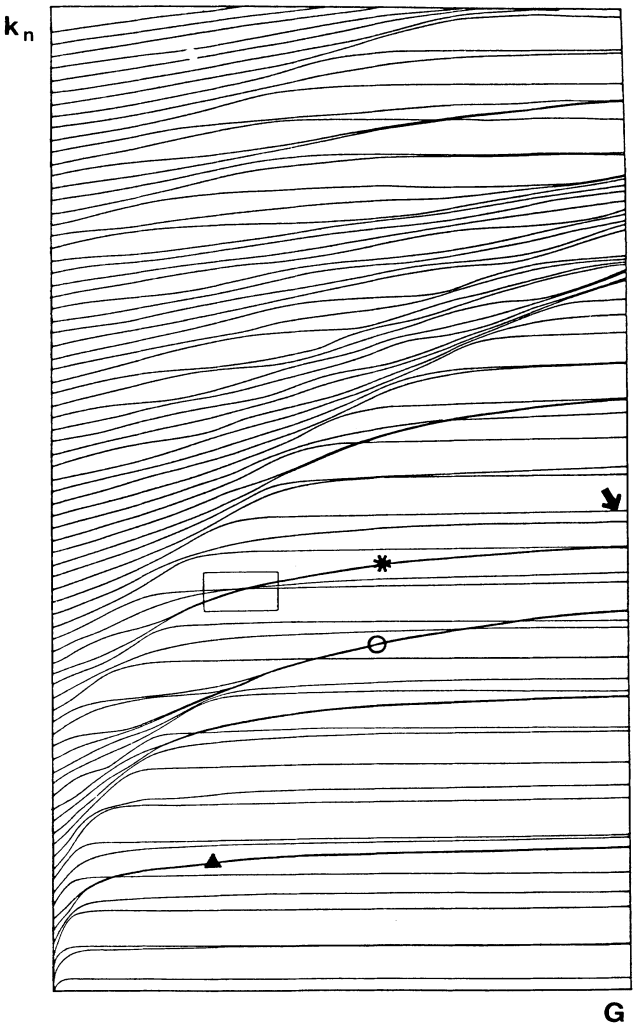

FIG. 2. The first 80 levels vs the effective coupling constant G ranging from 0 to 4000. Actually, we have plotted k_n/π instead of the energies E_n. Further explanations in main text.

thus making this particular rth factor almost zero. Only when $2(n \pm m)$ is close to 2×3^r or 4×3^r has the product a chance to yield an appreciable value. In other words, the matrix $H_{n,m}$ is essentially sparse, yet the off-diagonal matrix elements never tend to zero. This feature justifies truncation for numerical treatment as long as (i) the coupling G is not too large and (ii) one restricts oneself to the lower part of the spectrum.

In Fig. 2 we present part of the spectrum as obtained from matrix diagonalization. We are confident that the pattern displayed is not corrupted by the necessary truncation as the spectrum has been compared with the one obtained using Eq. (6). However, when using Eq. (6), only eight generations, i.e., 256 δ functions, have been effectively inserted into the square well. It is evident from Eqs. (3) that s generations should yield reliable results if one's interest is restricted to levels which obey $k_n \ll 3^s\pi$. In turn, matrix diagonalization of Eq. (10) automatically guarantees the limit $s \to \infty$, as long as errors inherent from truncation can be ruled out.

At the lower part of the spectrum the emergence of the limit $G \to \infty$ as indicated by Eqs. (3) is clearly discernable. While the twofold degeneracy at 9 (one level from $k_1^{(1)}/\pi$ and one from $k_0^{(2)}/\pi$) is attained, the fourfold degeneracy at 27 (above the single levels at 15, 18, and 21 on the right of Fig. 2) is only about to be attained. In fact, two closely lying levels marked by a triangle approach their limit at a slower rate than the other two on their top, which have virtually attained their limit for a lower value of the coupling constant. The marked levels undergo a typical avoided level crossing with the level which eventually reaches 21. Higher up this pattern repeats itself in a more and more dramatic way. A group of four levels marked by a circle, together with another two, marked by an asterisk, eventually approach the level at 81 (indicated by an arrow) to make up the eightfold degeneracy of that level. An appreciable number of avoided level crossings are generated from these clusters. The general pattern still higher up in the spectrum is that a level with its limit at 3^s for $G = \infty$ is approached for finite G by bunches of $2^{(s-2)}, 2^{(s-3)}, \ldots$ levels to make up the $2^{(s-1)}$-fold degeneracy of that level. In this way, avoided

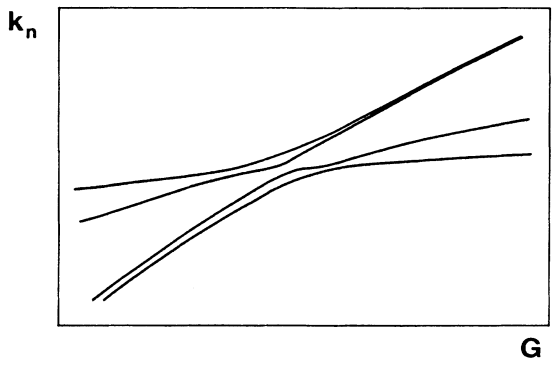

FIG. 3. A blown-up version of the section in the inset of Fig. 2.

level crossings occur on a larger and larger scale.

It is known that for finite-dimensional matrices genuine level crossings cannot occur if the matrix is irreducible with respect to internal symmetries.[12] We make the conjecture that in the model considered genuine level crossings are likewise excluded. The lines which appear to cross in Fig. 2 are in fact poorly resolved events of level repulsion. For demonstration we show in Fig. 3 a blown-up version of the section boxed in Fig. 2. It is further known that level repulsions are associated with the exceptional points of the Hamiltonian operator. The type of accumulated level repulsion encountered in our model strongly suggests that the distribution of spacings between pairs of neighboring eigenvalues is a Wigner distribution. Quantitative confirmation of this conjecture is in progress.

A possible extension of the model could be an investigation of the dependence on the Hausdorff dimension α, which means a more general choice of the Cantor set. Let r_1 and r_2 be positive numbers with $r_1+r_2<1$. A Cantor set $C(r_1,r_2)$ is then constructed as follows:

$$I_0=[0,1]\ ,$$

$$I_1=[0,r_1]\cup[1-r_2,1]\ ,$$

$$I_2=[0,r_1^2]\cup[r_1(1-r_2),r_1]\cup[1-r_2,1-r_2(1-r_2)]\cup[1-r_1r_2,1]\ ,$$

$$\cdots\ .$$

The set I_k is the union of 2^k disjoint compact intervals. A nonempty compact set of Lebesgue measure zero is then given by

$$C(r_1,r_2)=\bigcap_{k=0}^{\infty} I_k\ .$$

The set $C(r_1,r_2)$ has Hausdorff dimension α, with α being the unique root between 0 and 1 of the equation $r_1^\alpha+r_2^\alpha=1$. For $r_1=r_2=r$ it is $\alpha=\ln 2/\ln(1/r)$. In this paper $r=\frac{1}{3}$, i.e., $\alpha=0.63\ldots$, was considered.

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