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Finite discontinuities in the energy eigenvalue spectra of anharmonic oscillators

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Abstract. The existence of finite discontinuities in the energy eigenvalue spectra of certain multiterm potentials when their coupling parameters attain suitably chosen limiting values has been reported in the literature. We show that such discontinuities are also characteristic of such well-known systems as generalized anharmonic oscillators and the doubly anharmonic oscillator in one dimension. The present study strengthens the general conjecture that eigenvalue spectra are likely to display discontinuities in situations where a potential undergoes an abrupt change in shape with smooth variation of its coupling parameters.

Keywords. Anharmonic; double-well; discontinuity; eigenvalue spectra.

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1. Introduction

One can paraphrase a heuristic argument, originally put forward by Dyson (1952) to point to the breakdown of perturbation theory in the context of quantum electrodynamics, to claim that the energy eigenvalues of a multiterm potential $V(x)$ in quantum mechanics must necessarily be nonanalytic functions of the coupling parameter multiplying the term in the potential which is dominant in the limit $|x| \to \infty$. If λ be this coupling parameter and if the potential can support bound states for $\lambda \geqslant 0$ (binding being provided by a subdominant term in the potential at $\lambda = 0$), the potential will of necessity be unbounded from below for λ arbitrarily small and negative. Since power series converge in circles, it can be argued that the energy eigenvalues $E_n(\lambda)$ in such a case will not only be nonanalytic at $\lambda = 0$ but will also display an infinite discontinuity there (since the energy levels are finite for $\lambda \geqslant 0$ and drop to $-\infty$ for $\lambda = 0^-$). However as Herbst and Simon (1978) and Simon (1982) have pointed out with the help of counter examples, claims about the nonanalyticity of energy levels based on such arguments need to be treated with caution.

In addition to such infinite discontinuities, Calogero (1979) pointed out the possibility of the occurrence of finite discontinuities in energy eigenvalue spectra whenever the variation of the coupling parameters of a multiterm potential produced abrupt changes in the geometry of the associated potential wells. A detailed study of such discontinuities was reported by Saxena *et al* (1988) and Pandey and Varma (1989, 1990) for the generalized Killingbeck potential

$$V^{(1)}(r) = -1/r + 2\lambda r + 2\lambda^2 r^2$$

and the quark confinement potential

$$V^{(2)}(r) = 2\mu r + 2\lambda^2 r^2$$

($0 \leqslant r \leqslant \infty$). Discontinuous changes in the eigenvalue spectra were shown to exist whenever the geometry of the associated potential functions could be shown to change abruptly as λ was made to vanish and simultaneously μ was made to change sign.

In the present paper we wish to extend these studies of finite discontinuities in eigenvalue spectra to the case of the generalized anharmonic oscillators/double well potentials ($ax^2 + b^{k+1}x^{2k+2}$) where k is a natural number and $-\infty \leqslant x \leqslant \infty$, and to the doubly anharmonic oscillator ($ax^2 + bx^4 + cx^6$). We show that even these well studied potentials display such discontinuities in their eigenvalue spectra and we draw attention to the more unusual and interesting of such situations when the coupling parameters attain some suitably chosen limiting values.

2. The generalized anharmonic oscillator

Consider the generalized anharmonic oscillator potentials in one dimension:

$$V(x) = ax^2 + b^{k+1}x^{2k+2}, k = 1, 2, 3, \tag{1}$$

with $b > 0$ to ensure confinement. $V(x)$ as a function of x has a single minimum of zero depth at $x = 0$ for $a \geqslant 0$, but for $a < 0$ it has two symmetrically placed minima located at $x = \pm x_0$, where

$$x_0^2 = (|a|/((k+1)b^{k+1}))^{1/k}. \tag{2}$$

The depths of both the potential minima are equal and are given by

$$V(x_0) = -k(|a|/(k+1)b)^{1+1/k}. \tag{3}$$

Thus we can choose suitable paths in the space of real values of the parameters a and b such that the number of potential minima changes abruptly from one to two or vice versa with the new minima appearing or disappearing at $x = \pm\infty$ as a result of moving smoothly along these paths in parameter space. In such a case past experience would suggest that the energy eigenvalue spectrum should display finite discontinuity, whenever the minima that are created or destroyed are not infinitely deep.

To understand this better, consider the case of a potential with two minima. If one of these minima is wiped out as a result of a smooth variation of a control parameter, for quantum mechanical system this will not in general lead to a discontinuity in the energy spectrum because the system could ordinarily never have been completely localized within the potential minimum which was wiped out. A discontinuity would be expected to arise only when the variation of some control parameter either caused (i) a well defined minimum to arise or to be wiped out suddenly at an infinite distance away from the original minimum or caused (ii) an infinite barrier between the two minima to spring up or to vanish suddenly.

Returning to the consideration of the generalized anharmonic oscillators, to go from the situation of a single potential minimum to that of two minima, it is clear that the harmonic coupling a must change sign. An examination of (2) and (3) reveals that if the anharmonic coupling b is held fixed at a positive value then the two new wells that are created as the harmonic coupling a becomes negative, will be of zero depth and will be localized at $x=0$. Thus the change in the shape of the potential will be smooth and no discontinuity is to be expected in the energy spectrum. The energy eigenvalues of the system will pass smoothly into those of the pure x^{2k+2} oscillator as a vanishes and b is held constant and positive. Similarly if b is made to vanish while a is held fixed, for $a>0$ the energy eigenvalues will pass smoothly into those of the harmonic oscillator, while for $a<0$ they will collapse to $-\infty$ because the potential will now become unbounded from below at $b=0$.

Thus in order to observe a finite discontinuity in the energy spectrum it is necessary that b vanishes as a changes sign. We must also have $x_0^2 \to \infty$ and $V(x_0) \to$ constant in this limit for reasons discussed above. Let us therefore choose a as the control parameter and take

$$b=\mu|a| \tag{4}$$

where $\mu>0$, in which case (2) and (3) will read

$$x_0^2 = 1/((k+1)\mu^{k+1}|a|^k)^{1/k} \tag{5}$$

and

$$V(x_0) = -k/((k+1)\mu)^{1+1/k}. \tag{6}$$

Thus as a goes from 0^+ to 0^-, we go from a situation with a single well of zero depth at $x=0$ to two symmetrically placed wells of finite depth and infinite width located at $\pm\infty$, and as both couplings are vanishing together, all energy levels should collapse to zero at $a=0$ and should emerge all together from $-k/((k+1)\mu)^{1+1/k}$ – the bottom of the potential wells created at $\pm\infty$ as a turns negative. Also for $a\to 0^-$, the separation between the two wells which are symmetrically placed about the origin will grow to infinity, so that for all practical purposes the wells will become independent of each other. The eigenvalues should therefore show pairwise degeneracy as we make $a\to 0^-$.

We have used the method of scaled Hill determinants (Biswas *et al* 1971, 1973; Banerjee *et al* 1978) to calculate numerically the eigenvalue spectrum of the generalized anharmonic oscillators. Figure 1 shows the results of these calculations for $k=1$ and $\mu=0{\cdot}3$ and they are clearly in agreement with our analysis. We have also checked that the behaviour of the energy levels for other values of μ and k is similar.

3. The doubly anharmonic oscillator

Consider now the doubly anharmonic oscillator potential in one dimension:

$$V(x)=ax^2+bx^4+cx^6 \tag{7}$$

with $c>0$ to ensure confinement. The two dimensional parameter space of real values of the couplings a and b for fixed positive c can be divided into three regions:

Region I defined by

$$a>0, b>0$$

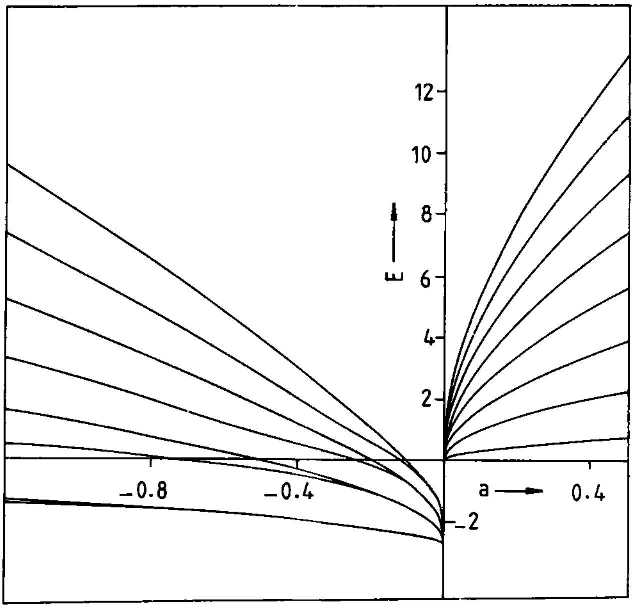

Figure 1. The energy eigenvalue spectrum of the potential $ax^2 + b^2x^4$ with $\mu = 0{\cdot}3$ plotted as a function of the coupling parameter a.

and

$$3ac > b^2, b < 0 \tag{8a}$$

is the region in which the potential possesses only one minimum which is of zero depth and is always located at $x = 0$.

Region II defined by

$$a < 0 \tag{8b}$$

is the region in which the potential possesses two minima symmetrically placed about the origin.

Region III defined by

$$a > 0, b < 0 \text{ and } 3ac < b^2 \tag{8c}$$

is the region in which the potential possesses three minima, one of which is always of zero depth and is located at the origin while the other two are symmetrically placed about it.

The two minima in the case of region II, and the two minima other than the one at the origin in region III are located at $x = \pm x_0$ where

$$x_0^2 = (\xi - b/|b|)|b|/3c, \tag{9}$$

and the value of the potential at both these minima is equal and is given by

$$V(x_0) = -(\xi - b/|b|)^2(2\xi + b/|b|)|b|^3/27c^2$$

where

$$\xi = (1 - 3ac/b^2)^{1/2}. \tag{10}$$

The situation, involving as it does three coupling parameters, is more complex than in the case of the generalized anharmonic oscillators. So we shall not attempt to be exhaustive, choosing instead to highlight the most interesting cases of the occurrence of finite discontinuities. Since we are interested in situations in which minima are created or destroyed at $x_0 = \pm\infty$, it is clear from (9) that we must consider the limit $c \to 0^-$. Since we also want $V(x_0)$ to show discontinuous changes, it is necessary that b changes sign as c vanishes. Thus there exist two possibilities: either both a and c vanish together as b changes sign or a is held constant as c vanishes and b changes sign.

Case I: $a, b, c \to 0$

To ensure that ξ remains real and that $V(x_0)$ remains finite while $x_0^2 \to \infty$, we take b as the control parameter and require that

$$a = \alpha |b|^{1/2}, c = \gamma |b|^{3/2} \text{ with } \gamma > 0. \tag{11}$$

For $a \geqslant 0$, we can ensure that we go from region I (one minimum) to region III (three minima) as b goes from positive to negative by choosing $3\alpha\gamma < 1$. The eigenvalue spectrum will look almost identical to that shown in figure 1 with the energy levels collapsing to zero as $b \to 0^+$ and emerging from a negative value which is equal to the depth of the potential wells created at $\pm\infty$ as b turns negative.

A somewhat more interesting situation exists for $a < 0$ i.e. $\alpha < 0$. Now from (10) $\xi > 1$ and for $b > 0$ we have

$$\begin{aligned} x_0^2 &\simeq (\xi - 1)/(3\gamma|b|^{1/2}) \\ V(x_0) &\simeq -(\xi - 1)^2(2\xi + 1)/(27\gamma^2) \end{aligned} \tag{12}$$

while for $b < 0$, we have

$$\begin{aligned} x_0^2 &\simeq (\xi + 1)/(3\gamma|b|^{1/2}) \\ V(x_0) &\simeq -(\xi + 1)^2(2\xi - 1)/(27\gamma^2). \end{aligned} \tag{13}$$

Now as b changes sign although the potential function always remains in the region of two minima, the location and depth of these minima change discontinuously. Consequently the energy levels will collapse (as all couplings vanish in the limit) to two different negative values corresponding to the two different values of $V(x_0)$ in the limits $b \to 0^+$ and $b \to 0^-$. The results of numerical calculations for $\alpha = -1$ and $\gamma = 1/8$ are shown in figure 2. They are clearly in agreement with the analysis presented above – the finite, adjustable discontinuity in the energy eigenvalue spectrum at $b = 0$ being evident.

Case II: $b, c \to 0, a > 0$

It is necessary to take $a > 0$ in order to provide confinement in the limit when both b and c vanish. All energy levels would collapse to $-\infty$ for both $b \to 0^+$ and $b \to 0^-$ if we were to choose $a < 0$. For $a > 0$, as b changes from positive to negative it is possible to move from region I to region III provided $3ac < b^2$. One way to ensure this is to choose $c = \gamma b^2, \gamma > 0$ with $3a\gamma < 1$. Now for $b > 0$, the potential has one minimum of zero depth at the origin, while for $b < 0$ there are two additional minima whose depth in the limit $b \to 0^-$ can be arranged to be zero provided we choose $a\gamma = 1/4$ so that $\xi = 1/2$ (for all other values of ξ, $V(x_0)$ will tend to $\pm\infty$ in the limit

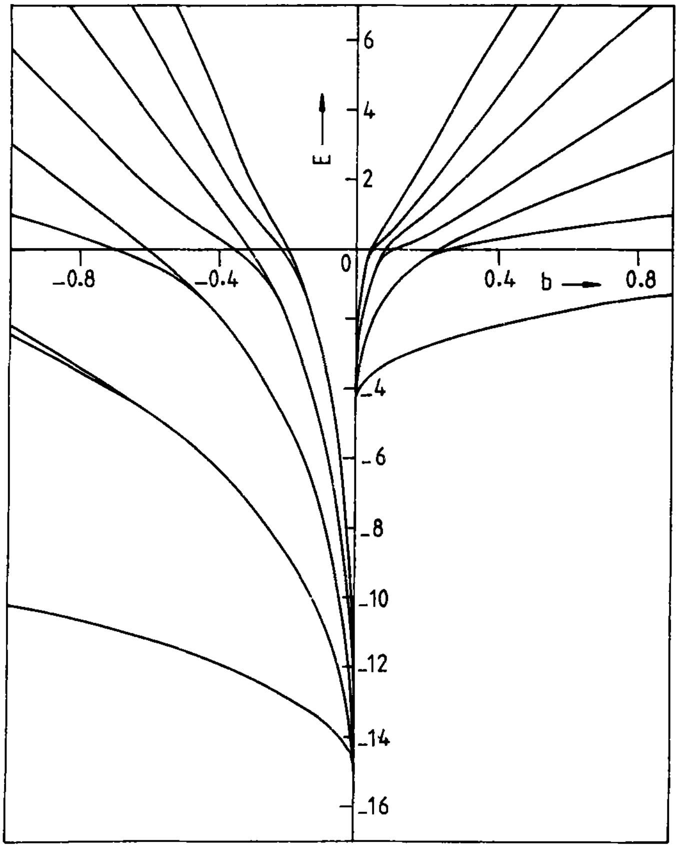

Figure 2. The energy eigenvalue spectrum of the potential $ax^2 + bx^4 + cx^6$ with $a = -|b|^{1/2}$, $c = |b|^{3/2}/8$ plotted as a function of the coupling parameter b.

$b \to 0^-$ so that either there will be no discontinuity at $b = 0$ or the discontinuity will be infinite).

The situation is therefore the following. As $b \to 0^+$, we have the harmonic oscillator energy spectrum $(2n+1)a^{1/2}, n = 0, 1, 2, \ldots$. But as b becomes negative by an infinitesimal amount, two new potential wells of zero depth are created at $\pm\infty$. Thus in the limit $b \to 0^-$ there is a harmonic oscillator well of zero depth at $x = 0$ characterized by the coupling constant a, and in addition there are two harmonic oscillator wells centered around $\pm x_0$ also of zero depth but each with coupling constant $4a$. Therefore the total spectrum as $b \to 0^-$ will be given by a set of nondegenerate levels characterized by the energies $(2n+1)a^{1/2}, n = 0, 1, 2, \ldots$ plus another set of doubly degenerate levels characterized by the energies $2(2m+1)a^{1/2}$, $m = 0, 1, 2, \ldots$. Actual numerical calculations for such a case for $a = 1$ are shown in figure 3 and the dramatic change in the spectrum at $b = 0$ is evident.

This is clearly the most interesting case of discontinuity in eigenvalue spectra encountered so far. The energy levels which can be identified with the central potential well are continuous across $b = 0$, however the energy levels associated with the two additional wells which occur at $\pm x_0$ for $b < 0$ first become degenerate as b approaches 0^- and then vanish completely for $b \geqslant 0$. It illustrates very graphically why

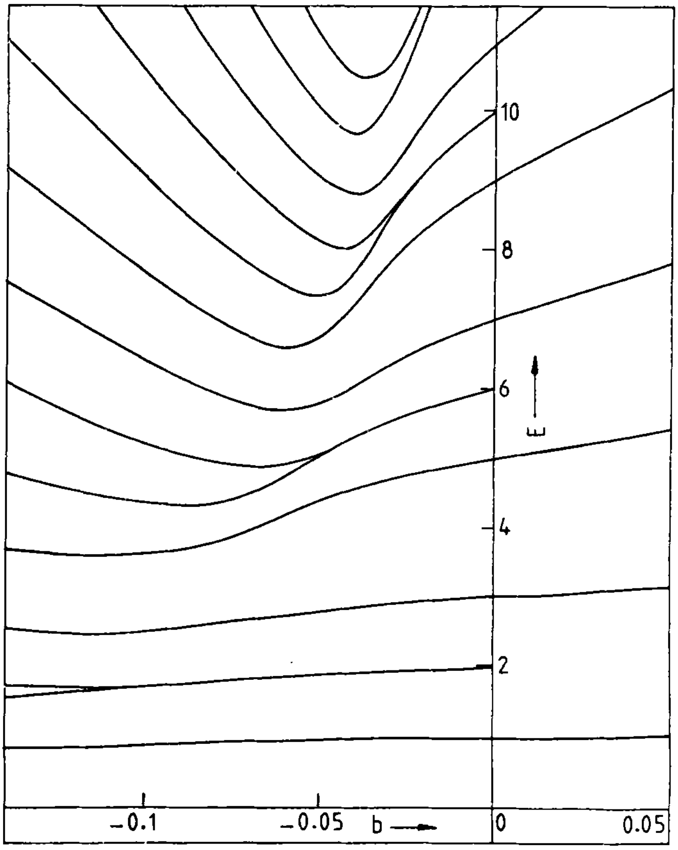

Figure 3. The energy eigenvalue spectrum of the potential $ax^2 + bx^4 + cx^6$ with $a = 1, c = b^2/4$ plotted as a function of the coupling parameter b.

perturbation series for the energy levels of the doubly anharmonic oscillator in powers of the coupling parameters are not ordinarily convergent.

4. Conclusion

In this paper we have reported on some of the hitherto unsuspected, rich diversity that exists in the energy eigenvalue spectra of the generalized anharmonic and the doubly anharmonic oscillators in one dimension. We have focussed our attention on the occurrence of finite discontinuities in the energy eigenvalue spectra when suitably chosen combinations of the couplings attain specific values. The existence of such discontinuities as revealed by our investigations points to the reason why perturbation expansions of the eigenenergy as power series of these couplings usually result in divergent or asymptotic series. The present study also confirms the finding of earlier investigations that multiterm potentials in general are likely to display discontinuous energy spectra whenever suitably selected combinations of the couplings in assuming chosen values produce abrupt changes in the geometry of the potential functions.

We would like to conclude with the following observation. We have seen that the energy eigenvalue spectrum of the potential $ax^2 + bx^4 + b^2x^6/4a$ for $a > 0$ undergoes a dramatic change as b changes sign (figure 3). If we consider an ensemble of non-interacting particles each moving in such a potential and immersed in a heat bath, the partition function can be easily calculated in the two limits $b \to 0^+$ and $b \to 0^-$ and they will be very different functions of the temperature of the heat bath. Therefore the thermodynamic properties of such an ensemble will show a discontinuous change across $b = 0$ pointing towards the existence of a phase transition. The implications of this observation are currently under investigation and details will be reported in a subsequent communication.

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