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Study of discontinuities in eigenvalue spectra of some model Hamiltonians

R K Pandey and V S Varma

Department of Physics and Astrophysics, University of Delhi, Delhi 110007, India

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Abstract. In this paper we study the eigenvalue spectra of two model s-wave Hamiltonians in three dimensions:

$$H = p^2/2 - 1/r + 2\mu r + 2\lambda^2 r^2$$

and

$$H = p^2/2 + 2\mu r + 2\lambda^2 r^2.$$

Using the method of Hill determinants we show that these eigenvalue spectra display discontinuities in the limit when both coupling constants μ and λ vanish simultaneously. We use a simple variational calculation to argue that such discontinuities are characteristic of these Hamiltonians and are not an artefact of our numerical methods. In fact, such discontinuities are also to be seen in the case of a displaced harmonic oscillator in one dimension whose eigenvalue spectrum is exactly solvable.

1. Introduction

Killingbeck (1978) noticed the remarkable property of the s-wave Hamiltonian

$$H = p^2/2 - 1/r + 2\lambda r + 2\lambda^2 r^2 \qquad 0 \leqslant r \leqslant \infty \tag{1}$$

that its exact ground-state wavefunction

$$\psi_0 = \exp(-r - \lambda r^2) \tag{2a}$$

becomes unnormalisable for negative values of λ, and therefore the corresponding solution of the ground-state energy

$$E_0 = -\tfrac{1}{2} + 3\lambda \tag{2b}$$

is valid only for $\lambda \geqslant 0$. This implies that the ground-state energy of this Hamiltonian, as a function of λ, is non-analytic at $\lambda = 0$, and so for $\lambda < 0$ E_0 must be a different function of λ than that given by equation (2b).

Later Calogero (1979) discussed a class of Hamiltonians of the form

$$H = p^2/2 + \frac{1}{2}\left(\frac{\partial \phi}{\partial x}(x, g) + \phi^2(x, g)\right) \qquad -\infty \leqslant x \leqslant \infty \tag{3}$$

where g is a coupling constant. He showed that these admit the exact ground-state wavefunction

$$\psi_0(x, g) = \exp\left(\int^x \mathrm{d}y\, \phi(y, g)\right) \tag{4}$$

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with the associated ground-state energy $E_0 = 0$. The form of $\phi(x, g)$ can be chosen such that $\psi_0(x, g)$ does not remain normalisable for all real values of the coupling constant g. Calogero considered specific examples of such Hamiltonians in which the exact ground-state wavefunction, although normalisable for all real non-zero values of g, became non-normalisable for $g = 0$ and showed that this loss of normalisability shows up as a discontinuity ($\lim_{g\to 0} E(g) \neq E(0)$) in the ground-state energy as a function of g. The non-analytic nature of the ground-state energy in such cases can also be understood by examining the behaviour of the corresponding potential $V(x, g) \equiv H - p^2/2$. Calogero pointed out that in all such cases the corresponding potential features wells whose locations move to infinity and whose depths remain constant or even diverge as the coupling constant approaches the value at which the discontinuity occurs.

Inspection shows that the Killingbeck Hamiltonian (1) is equivalent to the Calogero class of Hamiltonians in three dimensions with the corresponding $\phi(r)$ given by

$$\phi(r) = 1/r - 2\lambda r - 1 \tag{5}$$

and the ground-state wavefunction given by

$$\psi(r) = (1/r)\exp\left(\int^r \phi(s)\,\mathrm{d}s\right) \tag{6a}$$

$$= \exp(-r - \lambda r^2) \tag{6b}$$

which ceases to be normalisable as soon as λ becomes negative.

Saxena and Varma (1982) studied the Hamiltonian (1) and showed that the ground-state energy, although non-analytic, is in fact continuous across $\lambda = 0$, and they constructed the two different perturbation series in powers of $|\lambda|^{-1/2}$ which are valid for positive and negative λ. This, however, did not resolve the question of the general behaviour of the energy eigenvalues near $\lambda = 0$. More recently, Saxena *et al* (1988) showed by detailed numerical calculations, supported by a simple variational argument, that the energy spectrum as a whole possesses a discontinuity at $\lambda = 0$. Clearly for large $|\lambda|$, the $2\lambda^2 r^2$ term in the potential corresponding to the Hamiltonian (1) is dominant and the system behaves as a three-dimensional oscillator. As λ approaches 0+, their calculations showed that all the eigenvalues converge to the different s-wave hydrogen atom levels (since for $\lambda = 0$, $V(r) = -1/r$) but all emerge together from $-\frac{1}{2}$ as λ becomes negative. That is, all the energy levels except the ground state are discontinuous at $\lambda = 0$. This happens essentially because for all $\lambda \geq 0$ the potential possesses a single Coulomb-like minimum at the origin; but as λ becomes negative, even by an infinitesimal amount, the potential suddenly develops an infinitely wide additional minimum at $r_0 \simeq -1/2\lambda$ (i.e. infinitely far away from the origin) of depth $V_0 \simeq -\frac{1}{2} + 2\lambda$. All the energy levels (other than the ground state of the system) collapse into this well at infinity, in preference to the Coulomb-like well at the origin, as $\lambda \to 0-$.

In this paper we examine in detail the behaviour of the eigenvalue spectrum of a generalisation of the Hamiltonian (1) in which the coupling constants for the linear and quadratic terms are made independent of each other. The major thrust of this paper is to show that a discontinuity in the eigenvalue spectrum is characteristic of such Hamiltonians provided both coupling constants vanish simultaneously, and that the nature of the discontinuity depends upon the relationship between the two coupling constants as they vanish. The details of this analysis are presented in § 2, while in § 3 this analysis is repeated for the case in which the Coulomb term is missing from the

Hamiltonian to show that even in such a case the eigenvalue spectrum possesses discontinuities. All the numerical results reported in this paper are based on the method of Hill determinants (Biswas *et al* 1971, 1973). Finally in § 4 we discuss the implications of these results and provide an exactly solvable example whose eigenvalue spectrum displays a discontinuity of the kind discussed above.

2. Perturbed Coulomb interaction

We examine the s-wave eigenvalue spectrum of the Hamiltonian

$$H_1 = p^2/2 - 1/r + 2\mu r + 2\lambda^2 r^2 \tag{7}$$

which is an obvious generalisation of (1) to the case where the couplings of the linear and quadratic terms are made independent of each other. This has been done in order to elucidate the conditions under which discontinuities can appear in the eigenvalue spectrum associated with such Hamiltonians. Notice that the potential corresponding to this Hamiltonian can be written as

$$\begin{aligned} V_1(r) &= -1/r + 2\mu r + 2\lambda^2 r^2 \\ &= -1/r - \mu^2/2\lambda^2 + 2\lambda^2 (r + \mu/2\lambda^2)^2. \end{aligned} \tag{8}$$

It is clear that for $\mu < 0$ this potential possesses two minima, one of infinite depth at the origin (arising from the Coulomb term) and the other near

$$r_0 \simeq -\mu/2\lambda^2 \tag{9a}$$

of depth

$$V_1(r_0) = -\mu^2/2\lambda^2. \tag{9b}$$

However for $\mu \geqslant 0$ there is only the minimum at the origin, since $0 \leqslant r \leqslant \infty$.

Notice that the potential function given by equation (8) is similar to the classical potential which gives rise to a cusp catastrophe (Thom 1975). In the case of a classical particle a catastrophic transition from one potential minimum to another is observed when the minimum the particle is in initially is wiped out as a result of the variation of a control parameter. In the corresponding quantum mechanical situation no catastrophe would be observed, because the system could never be localised in one of its potential minima, unless the two minima were infinitely far apart or were separated by infinitely high barriers. Catastrophes, reflected as discontinuities in the energy spectra, are expected in quantum mechanical systems only when the variation of some control parameter either causes a well defined minimum to arise suddenly at an infinite distance away from the position of the original minimum, or causes an infinite barrier between two minima to vanish suddenly. Thus for the potential (8), discontinuities in the energy spectrum are likely to arise in the limit $\mu \to 0-$, only if $r_0 \to \infty$ simultaneously (i.e. the second minimum develops suddenly at ∞). This is possible only if we consider the limit in which both μ and λ tend to zero such that

$$\lambda = a|\mu|^b \tag{10}$$

where a and b are arbitrary positive constants which can be chosen appropriately. For $\mu < 0$ equations (9) can then be written as

$$r_0 \simeq -\mu^{(1-2b)}/2a^2 \tag{11a}$$

$$V_1(r_0) \simeq -\mu^{2(1-b)}/2a^2. \tag{11b}$$

Thus if we examine the behaviour of the potential around $\mu = 0$, it is clear that as μ changes sign, from positive to negative, we go abruptly from the situation in which the potential has a single minimum (at the origin) to one in which the potential has two minima (the position of the additional minimum being given by equation (11*a*)). The nature of this sudden change in the shape of the potential will be governed by our choice of the values of the constants a and b. Therefore it is of interest to investigate the behaviour of the eigenvalue spectrum of the Hamiltonian (7) for different choices of these constants.

2.1. The case $b = 1$

In this case equations (11) give, for $\mu < 0$,

$$r_0 \simeq -1/2\mu a^2 \tag{12a}$$

$$V_1(r_0) = -1/2a^2 + 2a^2\mu \tag{12b}$$

where we have included terms to order μ in equation (12*b*). These equations indicate that a well of constant depth $-1/2a^2$ and of infinite width develops at infinity as $\mu \to 0-$. Thus for all energy states which can be supported by this displaced harmonic well the preference is to be localised in this well at infinity rather than the much narrower Coulomb well at the origin. We therefore expect the energy levels to collapse to the bottom of this displaced well (i.e. $-1/2a^2$) as $\mu \to 0-$. On the other hand, those hydrogen atom levels which lie lower than the minimum of this displaced well will continue to remain localised in the Coulomb well. In this case, therefore, a can be adjusted to make the eigenvalues converge to any desired negative energy. In particular the eigenvalue spectrum for $a = \frac{1}{2}$, 1, $\frac{4}{3}$ and $\frac{5}{2}$ have been studied and the behaviour of the spectra match our expectations (figure 1). It is seen that if a is chosen such that the accumulation point ($-1/2a^2$) of the energy eigenvalues (as $\mu \to 0-$) is less than or equal to $-\frac{1}{2}$, all levels converge to this point ($-1/2a^2$ being equal to -2 in figure 1(*a*) and $-\frac{1}{2}$ in figure 1(*b*)). However, if this accumulation point is set such that it is greater than the ground-state energy ($-\frac{1}{2}$) but less than the first-excited-state energy ($-\frac{1}{8}$) of the s-wave hydrogen atom, the ground-state energy detaches itself from the accumulation point and becomes continuous across $\mu = 0$ while the other eigenvalues still collapse to the accumulation point ($-0.281\,25$ in figure 1(*c*) corresponding to $a = \frac{4}{3}$) as $\mu \to 0-$.

In order to confirm this picture of the behaviour of the energy spectrum we carry out a two-level linear variation calculation with the trial wavefunction given by

$$\psi = c_1 \exp(-r) + c_2 \exp[-a|\mu|(r + 1/2\mu a^2)^2] \tag{13}$$

which is a sum of two terms, the first of which is Coulomb-like at the origin while the other is harmonic oscillator-like but centred at $r_0 \simeq -1/2\mu a^2$. Neglecting terms (for $a < 2$, when $\mu < 0$) which vanish at least as fast as $\exp[(1-2/a)/4a|\mu|]$, the two eigenvalues are given by

$$E = -\tfrac{1}{2} - 3|\mu| + 6a^2\mu^2 \tag{14a}$$

$$E' = -1/2a^2 + (a-2)|\mu| + (13-5a)a^4\mu^2/2. \tag{14b}$$

We see that as $\mu \to 0-$, $E \to -\frac{1}{2}$ and $E' \to -1/2a^2$. As long as $-1/2a^2$ is less than (for $a = 0.5$ in figure 1(*a*)) or equal to $-\frac{1}{2}$ (for $a = 1$ in figure 1(*b*)), E' provides an upper bound to the ground-state energy whereas E provides an upper bound to the first-excited-state energy (MacDonald 1933). On the other hand, when $-1/2a^2$ becomes greater than $-\frac{1}{2}$ ($a = \frac{4}{3}$ in figure 1(*c*)), the upper bound on the ground-state energy is

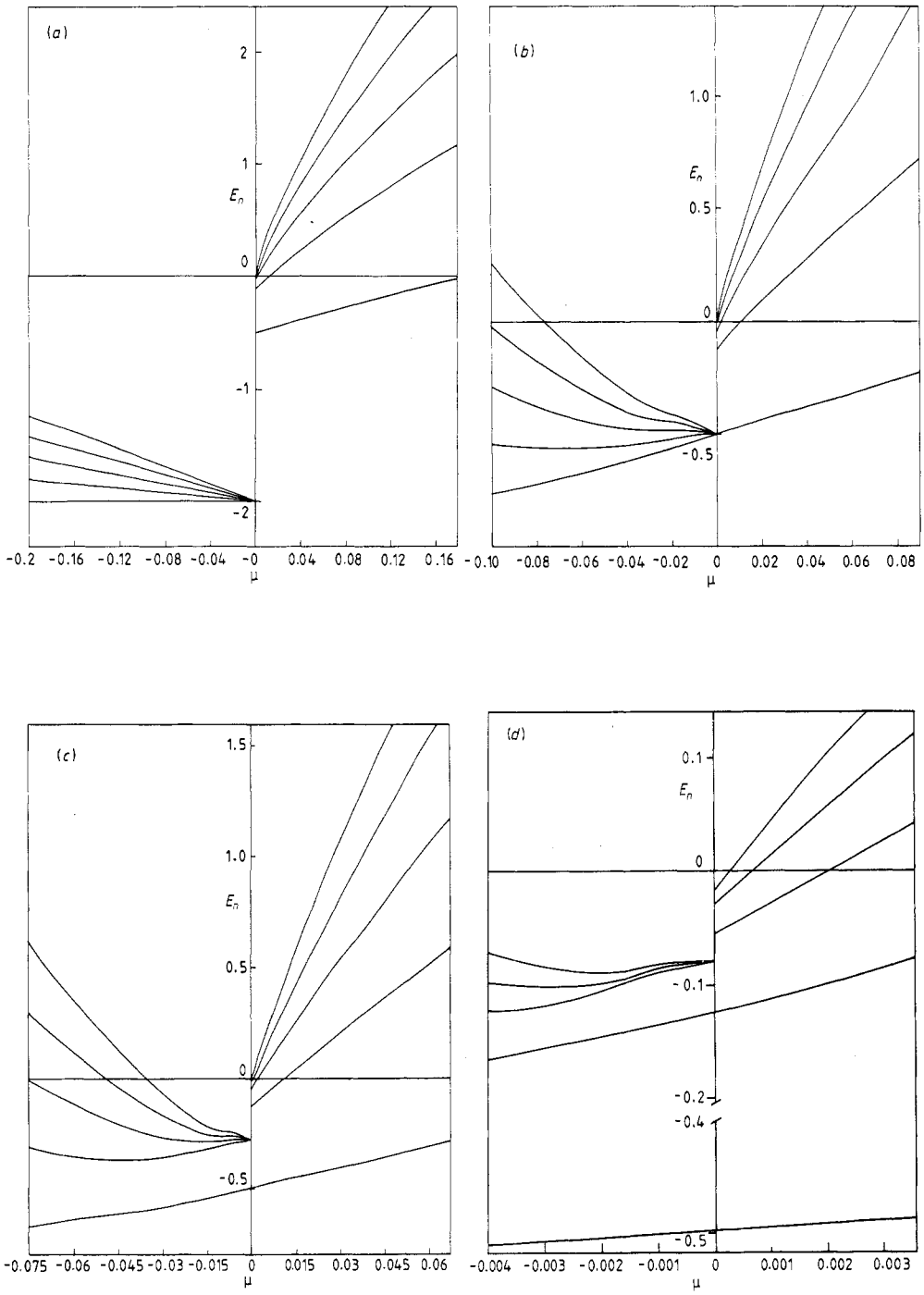

Figure 1. The energy spectra of the Hamiltonian H_1 plotted against μ for $b = 1$ and (a) $a = \frac{1}{2}$, (b) $a = 1$, (c) $a = \frac{4}{3}$ and (d) $a = \frac{5}{2}$.

provided by E which still remains at $-\frac{1}{2}$ as $\mu \to 0$ while E', which now lies higher than E, provides an upper bound on the first-excited-state energy. This therefore confirms the picture of the behaviour of the energy levels at their accumulation point in the limit $\mu \to 0-$ provided by our numerical calculations.

In fact, if we choose a value for a larger than 2 (say $a = 2.5$ in figure 1(d)) so that $-1/2a^2$ is set between the first- and second-excited-state energies of the s-wave hydrogen

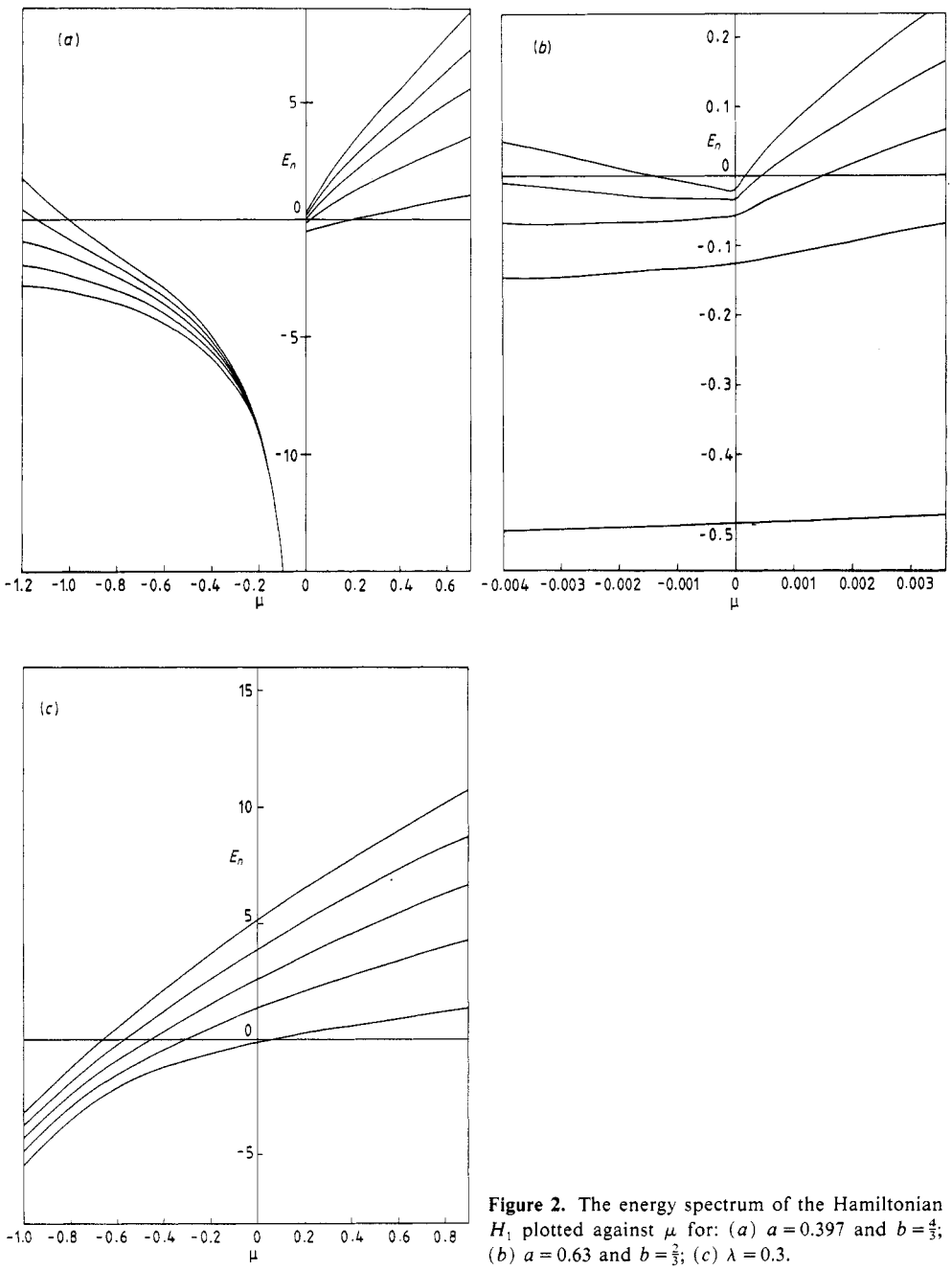

Figure 2. The energy spectrum of the Hamiltonian H_1 plotted against μ for: (a) $a = 0.397$ and $b = \frac{4}{3}$; (b) $a = 0.63$ and $b = \frac{2}{3}$; (c) $\lambda = 0.3$.

atom, the ground-state and the first-excited-state levels both detach themselves from the point of accumulation and become continuous across $\mu = 0$ since neither of these levels can now be supported by the well at infinity on account of it not being deep enough. The other levels still collapse to the accumulation point.

Therefore as the value of a is increased and the accumulation point is raised, one by one the energy levels detach themselves and become continuous across $\mu = 0$ with the s-wave hydrogen atom levels, until in the limit $a \to \infty$ the eigenvalue spectrum will show no discontinuity at all.

2.2. The case $b > 1$

Examination of equations (11) makes it clear that in this case the second minimum at infinity is infinitely deep, growing wider and wider as $\mu \to 0-$. Thus all the energy levels are expected to fall to $-\infty$ in the displaced harmonic well in the limit $\mu \to 0-$ independent of the value of a, while still converging to the s-wave hydrogen atom levels for $\mu \to 0+$. Figure 2(a) shows this type of discontinuity for $a = 0.397$ and $b = \frac{4}{3}$.

2.3. The case $b < 1$

We do not expect any discontinuity in the eigenvalue spectrum in this case since equations (11) indicate that the depth $V_1(r_0)$ of the second minimum tends smoothly to zero as $\mu \to 0-$, irrespective of the behaviour of r_0. The position of this well can be made to approach the origin for $b < 0.5$, can be fixed at a distance $r_0 \simeq 1/2a^2$ from the origin for $b = 0.5$ or can be made to go to infinity for $0.5 < b < 1$. However, since in each case the depth of the well tends to zero in the limit $\mu \to 0-$, all the eigenstates will remain confined in the Coulomb well in this limit and no discontinuity in the energy spectrum is expected for any value of a. We show that this is indeed the case for $a = 0.63$ and $b = \frac{2}{3}$ in figure 2(b).

2.4. The case λ = constant

Finally we consider the situation in which λ is kept at a fixed non-zero value and only μ is made to tend to zero. It can be verified from equation (9b) that this is another case in which the depth of the additional minimum tends to zero in the limit $\mu \to 0-$. We do not therefore expect any discontinuity in the eigenvalue spectrum and we see that this is indeed the case in figure 2(c) in which μ is varied across zero but λ is fixed at 0.3. Notice that as λ is never equal to zero the energy levels do not now coincide with the hydrogen atom levels at $\mu = 0$.

3. The three-dimensional oscillator

We now wish to discuss the behaviour of the s-wave energy spectrum of the Hamiltonian

$$H_2 = p^2/2 + 2\mu r + 2\lambda^2 r^2. \tag{15}$$

This Hamiltonian differs from our previous one in that the Coulomb term is missing. The reason for studying this Hamiltonian is to demonstrate explicitly that the discontinuities in eigenvalue spectra encountered in the previous section did not arise as a

result of the presence of the Coulomb term. The potential corresponding to this Hamiltonian can be written as

$$V_2(r) = 2\mu r + 2\lambda^2 r^2 \tag{16a}$$

or

$$V_2(r) = -\mu^2/2\lambda^2 + 2\lambda^2(r + \mu/2\lambda^2)^2. \tag{16b}$$

Clearly, for $\mu \geq 0$ this potential always has a minimum at the origin (since $0 \leq r \leq \infty$). However, for $\mu < 0$ the position r_0 and the depth $V_2(r_0)$ of its minimum are given by

$$r_0 = -\mu^{(1-2b)}/2a^2 \tag{17a}$$

$$V_2(r_0) = -\mu^{2(1-b)}/2a^2 \tag{17b}$$

where we have again taken

$$\lambda = a|\mu|^b \tag{17c}$$

since we wish to consider only the limit in which both μ and λ vanish simultaneously, as this is the situation in which a discontinuity in the energy spectrum is expected.

All the discussions of the previous section can be carried over except for the fact that as the Coulomb term is missing, all the eigenvalues are expected, in the limit $\mu \to 0+$, to tend to zero—the energy levels of a free particle.

3.1. *The case $b = 1$*

For $b = 1$, while all of the energy levels are expected to accumulate at zero as $\mu \to 0+$, they should, as $\mu \to 0-$, collapse to the bottom of the displaced harmonic well of depth $-1/2a^2$ which develops at ∞. Here a can be chosen to set the accumulation point of the energy eigenvalues to any desired negative energy as $\mu \to 0-$. In particular, the energy spectrum for $a = 1$ is shown in figure 3(a). The general behaviour of the spectrum in the limit $\mu \to 0-$ is similar to that discussed in the previous section.

3.2. *The case $b > 1$*

For values of b greater than one, as μ goes from positive to negative, a very wide well of infinite depth appears suddenly at infinity. Thus, in this case as $\mu \to 0-$ all eigenvalues are expected to collapse to $-\infty$. The qualitative behaviour of the energy spectrum in the region $\mu \geq 0$ is expected to remain the same as in the case $b = 1$ above. The eigenvalue spectrum for $a = 0.397$ and $b = \frac{4}{3}$ displaying these features is shown in figure 3(b).

3.3. *The case $b < 1$*

We do not expect any discontinuity in this case because the potential develops a minimum smoothly at the origin when μ becomes negative. The eigenvalues are thus expected to converge to zero in both limits $\mu \to 0-$ and $\mu \to 0+$. This feature of the energy spectrum is displayed in figure 3(c) for $a = 0.63$ and $b = \frac{2}{3}$.

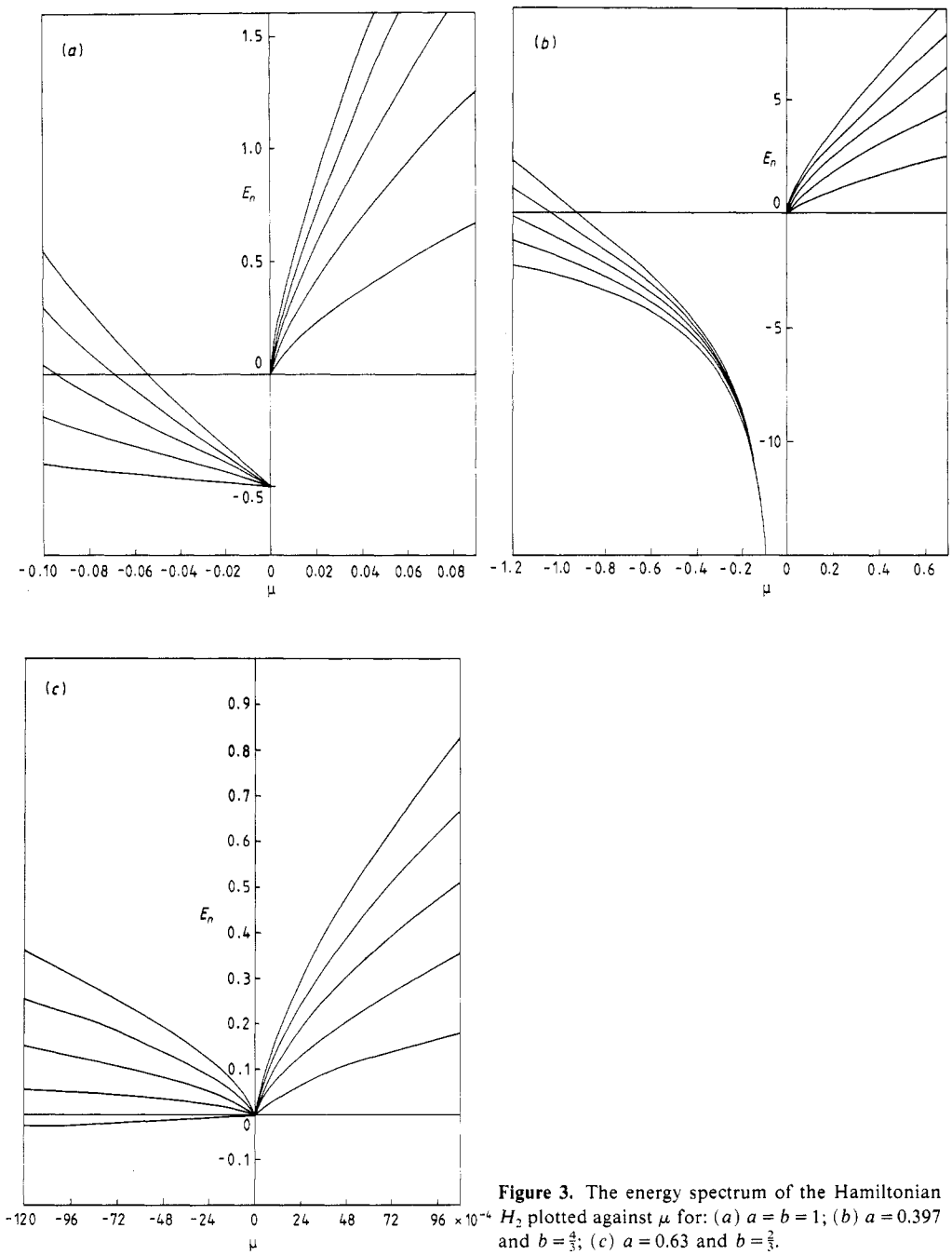

Figure 3. The energy spectrum of the Hamiltonian H_2 plotted against μ for: (*a*) $a = b = 1$; (*b*) $a = 0.397$ and $b = \frac{4}{3}$; (*c*) $a = 0.63$ and $b = \frac{2}{3}$.

4. Conclusion and the one-dimensional oscillator

We can summarise our findings by asserting that two conditions seem to be necessary for eigenvalue spectra to display discontinuity; a minimum of the potential should develop suddenly at infinity as some coupling constant or combination of coupling

constants crosses a critical value or a set of such values, and the depth of this minimum should be non-zero.

With the benefit of hindsight we can in conclusion offer a simple example for which analytic solutions are known and which displays most of the features we have studied. The example is nothing but the displaced harmonic oscillator in one dimension and is offered as evidence that our reported discontinuities in eigenvalue spectra are not artefacts of the numerical techniques we have used in this study. Consider therefore the one-dimensional Hamiltonian

$$H(x) = p^2/2 + 2\mu x + 2\lambda^2 x^2. \tag{18}$$

The corresponding potential function can be written as

$$\begin{aligned} V(x) &= 2\mu x + 2\lambda^2 x^2 \\ &= -\mu^2/2\lambda^2 + 2(\lambda x + \mu/2\lambda)^2 \end{aligned} \tag{19}$$

which has a minimum at

$$x_0 = -\mu/2\lambda^2 \tag{20a}$$

the depth of the minimum being

$$V_0 = -\mu^2/2\lambda^2. \tag{20b}$$

The eigenvalues of this system can easily be seen to be given by

$$E_n = -\mu^2/2\lambda^2 + (2n+1)|\lambda|. \tag{21}$$

These can be made to converge to any value between 0 and $-\infty$ in the double limit $\mu, \lambda \to 0$, whereas for μ and λ strictly equal to zero, all the E_n are always zero.

The analytic solutions of the one-dimensional displaced harmonic oscillator therefore display qualitatively the same features as we have established for Hamiltonians H_1 and H_2. This gives us confidence in our numerical results and shows that the discontinuities in eigenvalue spectra we have encountered are generic to the class of Hamiltonians we have studied.

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