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On the discontinuities in the energy spectrum of a model Hamiltonian

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Abstract. The occurrence of discontinuities in the energy spectrum of the s-wave Hamiltonian in three dimensions $H(\mu, \lambda) = p^2/2 - 1/r + 2\mu r + 2\lambda^2 r^2$ has been reported by us. In this communication we develop a unified understanding, based principally on the topography of the energy surfaces, of the different discontinuities we reported earlier. These discontinuities do not in general occur wherever the corresponding classical system would display catastrophic behaviour.

Keywords. Discontinuity; energy spectrum.

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1. Introduction

In a recent paper (Pandey and Varma 1988; hereafter referred to as I) we have reported the existence of discontinuities in the energy spectrum of the s-wave Hamiltonian in three dimensions

$$H(\mu, \lambda) = p^2/2 - 1/r + 2\mu r + 2\lambda^2 r^2. \tag{1}$$

These discontinuities were observed at $\mu = 0$ along the parametric curves

$$\lambda = a|\mu|^b \tag{2}$$

for all $b \geq 1$.

The Hamiltonian $H(\lambda, \lambda)$, i.e. with $\mu = \lambda$ in (1), was first studied by Killingbeck (1978), who pointed out that the ground state energy $E_0(\lambda, \lambda)$ was non-analytic at $\lambda = 0$. After careful numerical analysis, supported by a simple variation argument, Saxena *et al* (1988) succeeded in showing that apart from the ground state, the energy levels $E_n(\lambda, \lambda)$ as functions of λ are discontinuous across $\lambda = 0$. This behaviour of the energy spectrum was shown in I to be consistent with the criterion first enunciated by Calogero (1979), that discontinuities are likely to occur whenever the associated potential is such that it suddenly develops minima of non-zero depth even with smooth variation of some coupling constant.

Consider the potential function associated with the Hamiltonian (1),

$$\begin{aligned} V(r) &= -1/r + 2\mu r + 2\lambda^2 r^2 \\ &= -1/r - \mu^2/(2\lambda^2) + 2[\lambda r + \mu/(2\lambda)]^2. \end{aligned} \tag{3}$$

This potential develops, in addition to the Coulomb well at $r = 0$, an auxilliary harmonic oscillator-like well of depth $V_0 \simeq -\mu^2/(2\lambda^2)$ at $r_0 \simeq -\mu/(2\lambda^2)$ for $2\mu^3 + 27\lambda^4 < 0$. Thus in the limit $\mu, \lambda \to 0+$, $E_0(\mu, \lambda)$ always tends to $-1/2$—the ground state energy of the s-wave hydrogen atom. However, $E_0(\mu, \lambda)$ tends to the oscillator minimum $-\mu^2/(2\lambda^2)$ as $\mu \to 0-$ and $\lambda \to 0+$ whenever the depth of this minimum in this limit lies below $-1/2$. Therefore, on taking $\mu \to 0-$ along the parametric curves given by (2), it was shown in I that:

$$\text{i) for } b=1, \quad \lim_{\mu \to 0-} E_0(\mu, a|\mu|) = -1/(2a^2) \quad \text{for } a \leqslant 1$$
$$= -1/2 \quad \text{for } a \geqslant 1 \tag{4}$$

$$\text{ii) for } b>1, \quad \lim_{\mu \to 0-} E_0(\mu, a|\mu|^b) = -\infty \tag{5}$$

$$\text{iii) for } b<1, \quad \lim_{\mu \to 0-} E_0(\mu, a|\mu|^b) = -1/2. \tag{6}$$

Thus E_0 (μ, λ) has a discontinuity at the origin whenever the origin is approached along the curves given by (2) for $b \geqslant 1$.

In this paper we plot the energy surfaces $E_0(\mu, \lambda)$ and $E_1(\mu, \lambda)$ and show that they possess an infinitely deep cut all along the negative μ-axis. This cut arises from the fact that for $\lambda = 0$, the potential (3) becomes unbounded from below for $\mu < 0$ and is therefore non-confining for such values of μ and λ. Our purpose in this paper is (i) to develop a unified geometric understanding of the occurrence of the different discontinuities listed in (4)–(6) by showing that these arise purely from the topography of the energy surface $E_0(\mu, \lambda)$; and (ii) to draw attention to the fact that these discontinuities do not in general occur where the corresponding classical system would have displayed catastrophic behaviour.

2. The energy surface

We use the method of Hill determinants (Biswas *et al* 1971 and 1973) to calculate the ground state energy $E_0(\mu, \lambda)$ and in figure 1, we plot this energy surface as a function of μ and λ. The three most significant features of this plot, which are in fact characteristic of all $E_n(\mu, \lambda)$, are: i) The energy surface is symmetric about the μ axis. This follows from the fact that $H(\mu, \lambda)$ is an even function of λ. ii) The surface possesses an infinitely deep cut along the negative μ-axis. This is a consequence of the fact that the potential (3) is unbounded from below for $\lambda = 0$ and $\mu < 0$. iii) In any direction other than along the μ-axis, the energy surface rises linearly as $|\lambda|$ for $|\lambda| \to \infty$. This is because for large $|\lambda|$, the potential is dominated by the quadratic term $2\lambda^2 r^2$ and the system behaves like an s-wave three-dimensional harmonic oscillator.

Each of these features is evident in figure 1, but becomes even clearer if we look at the sections of the energy surface with planes of constant μ, λ and E. These are shown in figures 2, 3 and 4 respectively. We would like to draw special attention to the energy contours shown in figure 4, particularly to their behaviour near the origin. The feature worth noticing here is that the contour lines ($E_0 = \varepsilon$) are smooth curves for $\varepsilon \geqslant -1/2$ (recall that $-1/2$ is the ground state energy of the Coulomb well which survives for $\mu = \lambda = 0$). However, as soon as we consider $\varepsilon < -1/2$, the energy contours develop a cusp near the origin—the lip of the cusp getting narrower and longer as the

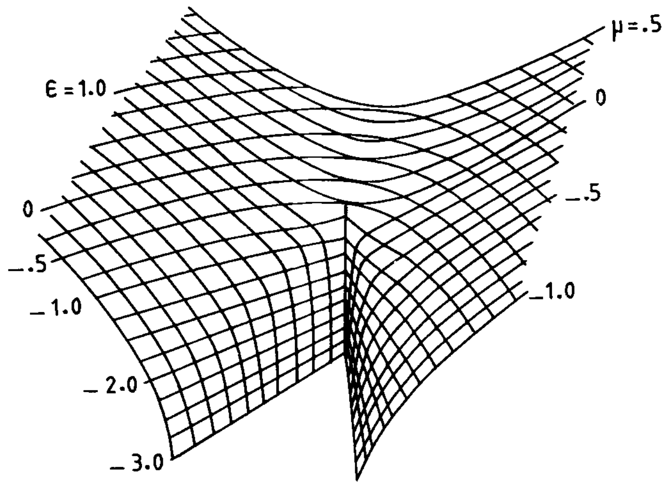

Figure 1. The ground state energy surface $E_0(\mu, \lambda)$ generated by plotting curves of constant energy $(-3{\cdot}0 \leqslant E_0 \leqslant 1{\cdot}5)$ and curves of constant μ $(-1{\cdot}0 \leqslant \mu \leqslant 0{\cdot}5)$.

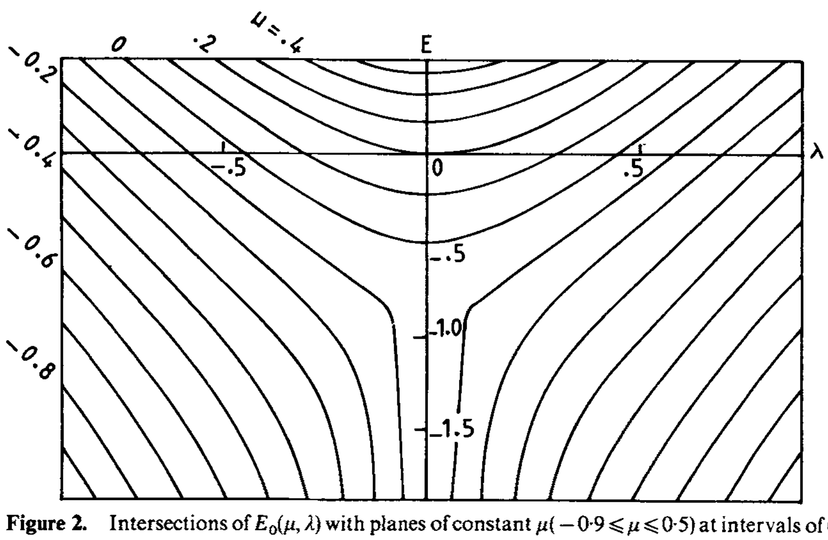

Figure 2. Intersections of $E_0(\mu, \lambda)$ with planes of constant $\mu(-0{\cdot}9 \leqslant \mu \leqslant 0{\cdot}5)$ at intervals of 0·1.

energy of the contour decreases. That this cusp develops suddenly for $\varepsilon < -1/2$, i.e. the slope $(\mathrm{d}\lambda/\mathrm{d}u)$ of the contour at the origin changes suddenly from infinity (for $\varepsilon = -1/2$) to 1 (in the limit $\varepsilon \to -1/2$ from below), is evident from the enlarged energy contour plots shown in figure 5. It is clear that the slope of an energy contour (for $\varepsilon < -1/2$) near the origin depends upon the energy of the contour. The contours come closer to the negative μ-axis as ε approches $-\infty$. Note that contours have not been drawn for $\varepsilon < -6{\cdot}0$ in figure 4 and $\varepsilon < -1{\cdot}2$ in figure 5, as they lie too close to each other and a wedge-like section around the negative μ-axis would have become black.

To summarize, if the energy contours for a fixed value of $E_0 = \varepsilon$ are given by the curves

$$\lambda = f_\varepsilon(\mu)$$

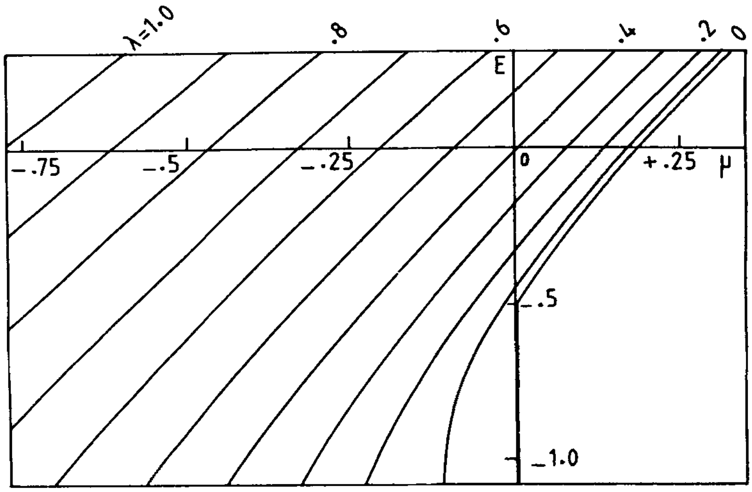

Figure 3. Intersections of $E_0(\mu, \lambda)$ with planes of constant $\lambda(-1{\cdot}0 \leqslant \lambda \leqslant 1{\cdot}0)$ at intervals of 0·1.

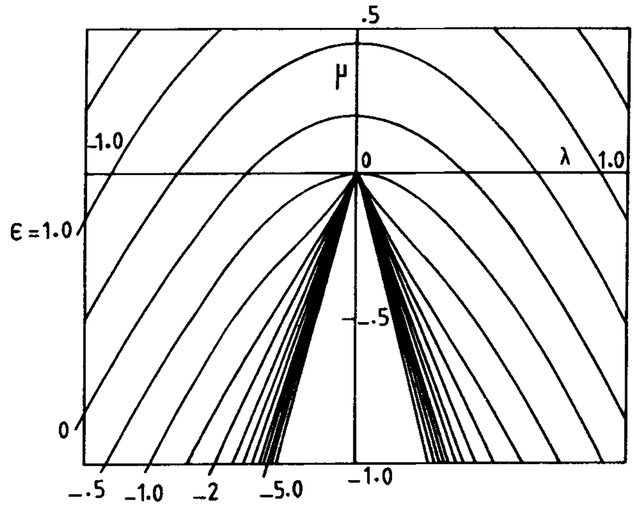

Figure 4. Contours of constant energy ε of the energy surface $E_0(\mu, \lambda)$ for $-6{\cdot}0 \leqslant \varepsilon \leqslant 1{\cdot}5$ plotted at intervals of 0·5.

with slopes

$$m_\varepsilon(\mu) \equiv \frac{\mathrm{d}f_\varepsilon(\mu)}{\mathrm{d}\mu}, \tag{7}$$

then i) for all $\varepsilon \geqslant -1/2$, $m_\varepsilon(\mu)$ is a continuous function of μ with

$$\lim_{\lambda \to 0} m_\varepsilon(\mu) = \infty, \tag{8}$$

i.e. tangents to the contours become parallel to the λ-axis along the line $\lambda = 0$.
ii) for $\varepsilon < -1/2$, the contours form a cusp at the origin, i.e. $m_\varepsilon(\mu)$ is analytic everywhere

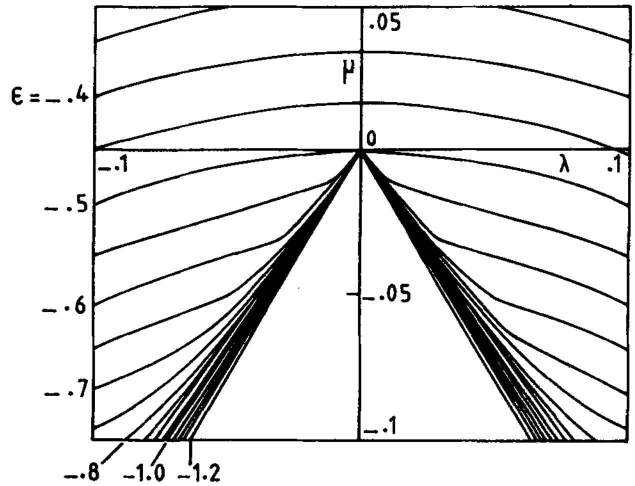

Figure 5. Contours of constant energy ε of the energy surface $E_0(\mu, \lambda)$ for $-1{\cdot}2 \leqslant \varepsilon \leqslant -0{\cdot}35$ plotted at intervals of 0·05 on an enlarged scale to display the behaviour near the origin.

Table 1. The slope $m_\varepsilon(0)$ at $\mu = \lambda = 0$ of a contour of energy $\varepsilon < -0{\cdot}5$ calculated from contour plots to show agreement with (9) in the text.

Contour of energy ε	λ for which line $\mu = -0{\cdot}005$ intersects contour	$\lvert m_\varepsilon(0)\rvert = \lambda/0{\cdot}005$	$1/(-2\varepsilon)^{1/2}$
−1·50	0·002887	0·5774	0·57735
−1·40	0·002988	0·5976	0·59761
−1·30	0·003101	0·6202	0·62017
−1·20	0·003228	0·6456	0·64550
−1·10	0·003372	0·6744	0·67420
−1·00	0·0035381	0·7076	0·70711
−0·90	0·0037306	0·7461	0·74536
−0·80	0·0039586	0·7917	0·79057
−0·70	0·0042347	0·8464	0·84515
−0·60	0·0045791	0·9158	0·91287

except at the origin, where

$$\lim_{\lambda \to 0\pm} m_\varepsilon(\mu) = \mp 1/(-2\varepsilon)^{1/2}. \tag{9}$$

The dependence of $m_\varepsilon(0)$ on ε given by (9) has been extracted from our numerical work. We list in table 1 the numerically evaluated slopes of the energy contours at the origin for values of $\varepsilon < -1/2$. We see that to a fair degree of accuracy the results are consistent with (9).

The change in the behaviour of the energy contours near the origin for $\varepsilon < -1/2$ is a consequence of the fact that a ground state of energy less than $-1/2$ cannot be supported by the Coulomb well and can only be localized in the subsidiary harmonic oscillator well centred at $r_0 \simeq -\mu/(2\lambda^2)$ whenever the minimum of this well $\simeq -\mu^2/(2\lambda^2)$

drops lower than $-1/2$. In such a case in the limit $\mu \to 0-$, $\lambda \to 0$, as the well becomes infinitely wide, the ground state energy of the system collapses to the bottom of the well and $\varepsilon = -\mu^2/(2\lambda^2)$, i.e. $\lambda = \pm\mu/(-2\varepsilon)^{1/2}$, so that

$$(\partial\lambda/\partial\mu)|_\varepsilon = \pm 1/(-2\varepsilon)^{1/2}$$

which agrees with (9) which was established numerically. Thus the behaviour of the energy contours embodied by (9) provides additional evidence for the localization of the ground state of the system in the subsidiary oscillator well which developes at $r=\infty$ in the limit $\mu \to 0-$ and $\lambda \to 0$ in preference to the Coulomb well at $r=0$.

The discontinuous behaviour of the energy contours near the origin given by (8) and (9) holds the key to the understanding of the discontinuities in the ground state energy given by (4) and (5) above.

3. Geometry of the discontinuities

Having described the topography of the ground state energy surface, let us now see how a section of the energy surface by another smooth surface can show discontinuity.

Consider therefore a family of surfaces S which contain the energy axis and are everywhere normal to the (λ, μ) plane. A surface belonging to this family can be specified by the equation of the curve of its intersection with the (λ, μ) plane. Let us choose this to be given by (2). Then the slope m_s of these curves, defined by

$$m_s(\mu) \equiv \frac{d\lambda}{d\mu} = ab\mu^{b-1} \tag{10}$$

is at $\mu=\lambda=0$ equal to a for $b=1$, zero for $b>1$ and infinite for $b<1$. Consider now the intersection of the energy surface $E_0(\mu, \lambda)$ with such surfaces S. For $\mu>0$, independent of the value of $m_s(0)$, as μ and thus λ tends to zero, the surfaces S always intersect the contour of energy $\varepsilon = -1/2$ at the origin. However for $u \to 0-$, because of the presence of the cusp the situation depends upon the value of $m_s(0)$. So long as $|m_s(0)| \geqslant 1$, the surfaces S still intersect the contour of energy $\varepsilon = -1/2$ at the origin and the curves of intersection of $E_0(\mu, \lambda)$ with S are continuous across $\mu=\lambda=0$. But for $|m_s(0)| < 1$, the contour ε that a particular surface S intersects at the origin is the one whose tangent has a slope $m_\varepsilon(0) = m_s(0)$. Thus from (9) and (10) it follows that the energy of the contour intersected by S in the limit $\mu \to 0-$ is

$$\begin{aligned} &\varepsilon = -1/(2a^2) && \text{for } b=1 \text{ and } a \leqslant 1 \\ &\varepsilon = -\infty && \text{for } b>1 \\ &\varepsilon = -1/2 && \text{for all other } a, b. \end{aligned} \tag{11}$$

These observations serve to explain completely the discontinuities in the ground state energy that were reported in *I*. By way of illustration we show in figures 6a and 6b the intersection of $E_0(\mu, \lambda)$ with the surfaces S for $b=1$ and $a=1$, $a=1/\sqrt{3}$ respectively. Consistent with our analysis, the curve of intersection is continuous across the origin in the first case, and shows a clear discontinuity in the second.

Our analysis also shows that as $E_0(\mu, \lambda)$ has an infinitely deep cut along the negative

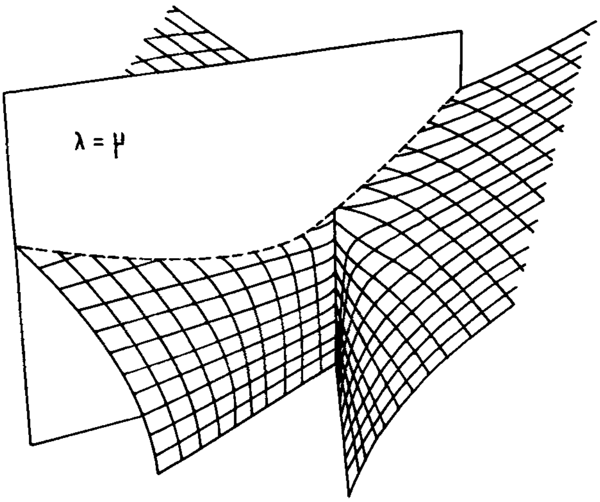

Figure 6a. Intersection of the energy surface $E_0(\mu, \lambda)$ with the plane normal to the (λ, μ) plane and characterized by $\lambda = \mu$ showing no discontinuity.

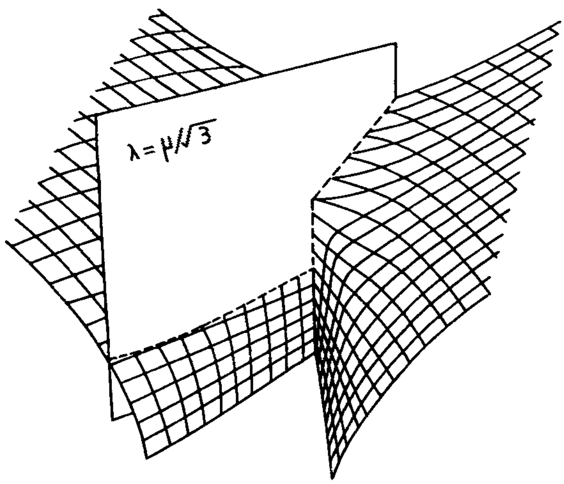

Figure 6b. Intersection of the energy surface $E_0(\mu, \lambda)$ with the plane normal to the (λ, μ) plane and characterized by $\lambda = \mu/\sqrt{3}$ showing discontinuity along the energy axis.

μ-axis, its section with any surface which crosses the μ-axis for $\mu < 0$ will be a curve which tend to $-\infty$ as $\lambda \to 0$.

4. Conclusion

In this paper we have shown how the discontinuities in the ground state energy reported in I, can be understood in terms of the topography of the energy surface resulting essentially from its structure near the origin and the presence of an infinitely

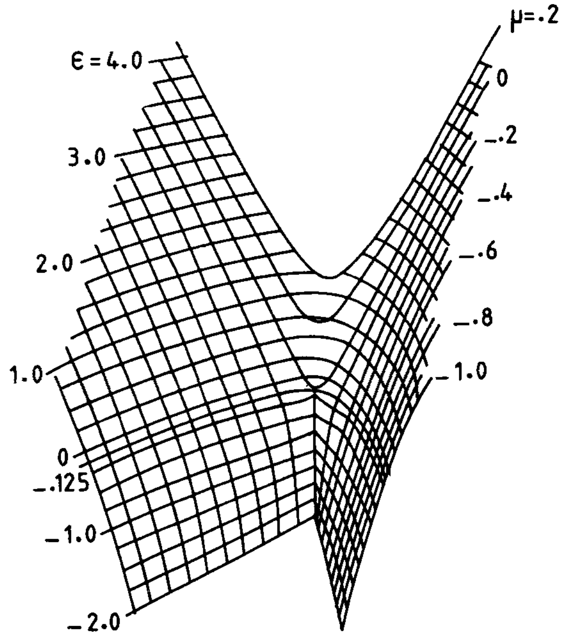

Figure 7. The first excited state energy surface $E_1(\mu, \lambda)$ generated by plotting curves of constant energy $(-2.0 \leqslant E_1 \leqslant 4.0)$ and curves of constant $\mu(-1.0 \leqslant \mu \leqslant 0.2)$.

deep cut along the negative μ-axis. Since the energy surfaces corresponding to the excited states are topographically similar (we display in figure 7 the first excited state by way of illustration) the analysis presented above can be applied *mutatis mutandis* to the excited states, where similar results hold.

The major result for the excited states is that the nth energy level will display discontinuity at $\mu = \lambda = 0$ if the depth of the subsidiary minimum that develops as $\mu \to 0-$ and $\lambda \to 0$ lies lower than the nth energy level of the Coulomb potential. In other words this means that the nth energy level will be discontinuous across the origin along all paths $\lambda = f(\mu)$ with slope at the origin $(\mathrm{d}\lambda/\mathrm{d}\mu)|_0 < (n+1)$.

For those familiar with classical systems displaying catastrophic behaviour (cusp catastrophe, Thom (1973)), it is worth remarking that the energy surface in general displays no discontinuity across the curve $2\mu^3 + 27\lambda^4 = 0$ which separates the region where the potential function (3) has one minimum (the Coulomb minimum at the origin) from the region where it has an additional minimum in the physical region $0 \leqslant r \leqslant \infty$. For a classical system, this equation marks the boundary of the bifurcation set across which the system can display catastrophic transitions. Our work has demonstrated that the corresponding quantum mechanical system displays catastrophe only across the origin ($\mu = \lambda = 0$) and not anywhere else across the classical boundary. The reason that the energy of our quantum mechanical system displays no discontinuity everywhere across the boundary of the classical bifurcation set has to do with the fact that in a situation with two potential wells, a quantum system in a stationary state can never be considered to be completely localized in any one of the wells—the wavefunction stretches over all r, unless the wells are either separated by infinitely high walls or one of the wells is infinitely wide in comparison to the other. Since in the present case the wells are never separated by infinitely high walls and the additional oscillator-like well is never infinitely wide except in the limit $\lambda \to 0$, $\mu \to 0-$, the energy surface displays no discontinuity across the boundary of the corresponding classical bifurcation set except at $\mu = \lambda = 0$.

Although in our analysis we have always considered the *s*-wave Hamiltonian, the behaviour of the energy spectra for $l \neq 0$ is not expected to be qualitatively different. Even though as a result of the presence of the centrifugal barrier for $l \neq 0$, the potential function goes to $+\infty$ instead of $-\infty$ at $r=0$, the combination of $l(l+1)/r^2$ and $-1/r$ gives rise to a minimum near the origin which is deep enough to support the ground state which now has an energy $-1/(2(l+1)^2)$. The total potential function (including the $2\mu r + 2\lambda^2 r^2$ terms) will still be non-confining for $\lambda = 0$ and $\mu < 0$ and will still develop a subsidiary oscillator-like well at $r = \infty$ when we take the limit $\lambda \to 0$, $\mu \to 0-$ along the parametric curves given by (2). Discontinuities similar to the ones reported in this paper will now develop when the ground state energy drops below $-1/(2(l+1)^2)$ rather than below $-1/2$ as happens for $l = 0$.

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