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LETTER TO THE EDITOR

An example of a quantum catastrophe

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Abstract. We study the excited-state energies of the s-wave hydrogen atom with the polynomial perturbation $2\lambda r+2\lambda^2 r^2$. We demonstrate the existence of a discontinuity in the eigenvalue spectrum at $\lambda=0$ as λ changes from positive to negative.

The ground state of the s-wave Hamiltonian for a hydrogen atom with a polynomial perturbation

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

was first studied by Killingbeck (1978). Such Hamiltonians are also of interest in studies of quark confinement where the $-1/r$ term represents the gluon exchange potential and the $2\lambda r+2\lambda^2 r^2$ terms are responsible for confinement. Killingbeck pointed out that for $\lambda>0$ this Hamiltonian possesses the exact solution for the ground state given by

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

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

Although these are acceptable as the ground-state energy and wavefunction respectively for $\lambda>0$, they are clearly unacceptable for $\lambda<0$ since then ψ_0 becomes non-square integrable. Thus the usual Rayleigh-Schrödinger (RS) perturbation theory in powers of λ for the ground-state energy, which agrees with (2*a*), clearly breaks down for $\lambda<0$. Subsequently it was shown by Saxena and Varma (1982) from arguments based on scaling that the correct expansion parameter for the RS series in the present case is $|\lambda|^{-1/2}$ and not λ and this leads, for the ground-state energy, to the perturbation expansion for large $|\lambda|$:

$$E_0=3|\lambda|+(8|\lambda|/\pi)^{1/2}(\lambda/|\lambda|-1)+[\tfrac{3}{2}-(8\ln 2)/\pi]+(\lambda/|\lambda|)[(8\ln 2)/\pi-2]+\ldots \tag{3}$$

which is non-analytic at $\lambda=0$ and gives different series for positive and negative λ. It agrees with (2*a*) for $\lambda>0$ and its correctness for $\lambda<0$ for large $|\lambda|$ was verified by variational and Hill determinant calculations.

In this letter we study the behaviour of the energy levels of the excited states of the Hamiltonian (1) as a function of λ. We start with a qualitative discussion. Note that, for large $|\lambda|$, the Hamiltonian (1) is dominated by the $2\lambda^2 r^2$ term. Hence it is easy to see that

$$\lim_{|\lambda|\to\infty} E_n=(4n+3)|\lambda| \qquad n=0,1,2,\ldots \tag{4}$$

and these are in fact upper bounds to the energy levels of the system for negative λ since $H<p^2/2+2\lambda^2 r^2$ for $\lambda<0$.

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The behaviour near $\lambda = 0$ is much more complicated. To see this we write the potential corresponding to the Hamiltonian (1) as

$$V(r) = -1/r + 2\lambda r + 2\lambda^2 r^2 = -1/r - \tfrac{1}{2} + 2(\lambda r + \tfrac{1}{2})^2. \tag{5}$$

Thus as $\lambda \to 0^+$ the potential goes smoothly into the attractive Coulomb potential $-1/r$. Therefore in this limit the eigenvalues should tend smoothly to the s-wave hydrogen atom eigenvalues:

$$\lim_{\lambda \to 0^+} E_n = -1/[2(n+1)^2] \qquad n = 0, 1, 2, \ldots. \tag{6}$$

Since in fact the terms $2\lambda r$ and $2\lambda^2 r^2$ are positive definite for $\lambda > 0$, the hydrogen atom eigenvalues provide lower bounds to the energy levels for all positive λ.

However, for negative λ, in addition to the attractive Coulomb well at $r = 0$, the potential possesses a subsidiary minimum at $r \simeq -1/2\lambda$, of width $\simeq -1/2\lambda$ and depth $\simeq 2\lambda - \frac{1}{2}$. Thus in the limit $\lambda \to 0^-$, the position of this subsidiary minimum moves to infinity, its width also becomes infinite and its depth tends to the constant value $-\frac{1}{2}$. Therefore, in this limit, other than the ground state of the stystem $-\frac{1}{2} - 3|\lambda|$ which remains localised in the Coulomb well, all other states collapse preferentially into the displaced harmonic oscillator well at $r = 1/2|\lambda|$. The expected behaviour of the eigenvalues is therefore

$$\lim_{\lambda \to 0^-} E_n = -\tfrac{1}{2} + (2n-3)|\lambda| \qquad n = 0, 1, 2, \ldots \tag{7}$$

i.e. all the eigenvalues collapse to $-\frac{1}{2}$ and the slope of the nth eigenvalue for $\lambda \to 0^-$ is expected to be $-2n+3$.

To summarise, for $\lambda > 0$ the system possesses a Coulomb well at the origin and an infinite confining wall which moves further and further away as $\lambda \to 0$. At $\lambda = 0$, only the Coulomb well remains and the energy spectrum transforms smoothly to that of a s-wave hydrogen atom. Then as soon as λ becomes negative, even by an infinitesimal amount, a very wide harmonic oscillator well springs up at $-1/2\lambda$ whose depth is equal to the energy of the ground state of the hydrogen atom. The spectrum thus transforms from equation (6) at $\lambda = 0$ to equation (7) for $\lambda < 0$. There is therefore a discontinuity in the behaviour of the energy levels at $\lambda = 0$ as we go from positive to negative λ. They go into the different Coulomb levels $-1/[2(n+1)^2]$ at λ equal to zero and emerge all together from $-\frac{1}{2}$ as λ becomes negative. The possibility of discontinuity in the eigenvalue spectrum may also be seen to arise from the fact that the surface of extrema of the potential $V(r)$ given by equation (5) can be written as

$$M = r(1/r^3 + 2\lambda/r + 4\lambda^2) = (z^3 + 2\lambda z + 4\lambda^2)/z \qquad \text{for } z = 1/r$$

where the expression within brackets is reminiscent of the classical catastrophe (Thom 1975). However, the differences need to be noted. In the present case the coefficients of the constant and linear terms are not independent of each other, the range of variation of z is only over the positive real line, and the surface of extrema possesses additional structure because of the presence of z in the denominator.

To put these qualitative arguments regarding the behaviour of the eigenvalue spectrum on a firm footing we carry out a two-parameter linear variational calculation for $\lambda < 0$, using as our trial wavefunction:

$$\psi_t(r) = C_1 \exp(-r) + C_2 \exp[\lambda(r + 1/2\lambda)^2] \tag{8}$$

the first term representing the ground-state wavefunction of a Coulomb potential and the second the ground-state wavefunction of a displaced harmonic oscillator centred at $r=-1/2\lambda$ (remember $\lambda<0$). If we ignore terms which vanish as fast as or faster than $\exp(1/4\lambda)$ in the limit $\lambda\to 0^-$, the secular determinant is diagonal and the system has two levels:

$$E_0=-\tfrac{1}{2}+3\lambda+6\lambda^2 \qquad E_1=-\tfrac{1}{2}+\lambda+4\lambda^2. \tag{9}$$

These therefore provide upper bounds to the ground-state and the first excited-state energy levels of the system for negative λ (MacDonald 1933), showing that neither of these levels can lie higher than $-\frac{1}{2}$ in the limit $\lambda\to 0^-$.

We now use the method of Hill determinants (Biswas *et al* 1971, 1973) to calculate numerically the eigenvalues of the system. For this purpose we use an ansatz for the wavefunction given by

$$\psi(r)=\exp(-\alpha r-|\lambda|r^2)\sum_{n=0}^{\infty}a_n r^{n+\sigma} \tag{10}$$

where α is an adjustable parameter included to ensure convergence and σ is the positive root of the indicial equation in a standard Fuch's type solution (Copson 1935) of the Schrödinger equation corresponding to the Hamiltonian H. The numerical values of the first four eigenvalues of the system for $-0.1\leqslant\lambda\leqslant 0.1$ are listed in table 1, and the behaviour of the first nine eigenvalues for $-0.5\leqslant\lambda\leqslant 0.5$ is shown graphically in figure 1. The catastrophic collapse of the eigenvalues to $-\frac{1}{2}$ from the left of $\lambda=0$ and their emergence from the s-wave hydrogen atom levels from the right is clearly seen.

Table 1. The results of the calculations of the first four eigenvalues of the Hamiltonian (1) to six significant places for $-0.1\leqslant\lambda\leqslant 0.1$ using the method of Hill determinants.

	E_0	E_1	E_2	E_3
+0.10	−0.200 000	0.803 302	1.497 085	2.110 760
+0.09	−0.230 000	0.717 643	1.358 972	1.922 717
+0.08	−0.260 000	0.631 234	1.219 370	1.732 596
+0.07	−0.290 000	0.543 951	1.078 012	1.540 012
+0.06	−0.320 000	0.455 632	0.934 536	1.344 442
+0.05	−0.350 000	0.366 057	0.788 434	1.145 144
+0.04	−0.380 000	0.274 908	0.638 953	0.941 007
+0.03	−0.410 000	0.181 703	0.484 883	0.730 208
+0.02	−0.440 000	0.085 622	0.324 019	0.509 352
+0.01	−0.470 000	−0.014 973	0.151 347	0.270 358
0.00	−0.500 000	−0.125 000	−0.055 556	−0.031 250
−0.01	−0.530 000	−0.510 432	−0.490 895	−0.471 394
−0.02	−0.560 000	−0.521 895	−0.484 162	−0.446 988
−0.03	−0.589 997	−0.534 759	−0.481 084	−0.428 384
−0.04	−0.619 882	−0.548 281	−0.476 473	−0.399 587
−0.05	−0.649 107	−0.558 996	−0.462 748	−0.356 282
−0.06	−0.676 826	−0.564 684	−0.440 225	−0.302 607
−0.07	−0.702 453	−0.565 311	−0.410 802	−0.241 233
−0.08	−0.725 788	−0.561 518	−0.275 910	−0.173 812
−0.09	−0.746 866	−0.553 969	−0.336 551	−0.101 457
−0.10	−0.765 827	−0.543 211	−0.293 450	−0.024 969

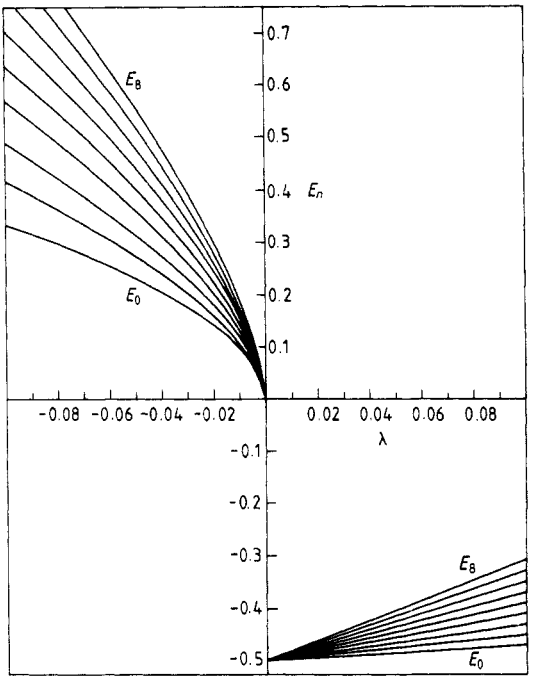

Figure 1. Plot of the first nine eigenvalues of the Hamiltonian (1) for $-0.5 \leq \lambda \leq 0.5$ calculated using the method of Hill determinants.

As a matter of interest, we look at the eigenvalue spectrum of the Hamiltonian

$$H_R = p^2/2 + 1/r - 2\lambda r + 2\lambda^2 r^2 \tag{11}$$

which differs from H in that the Coulomb term is now repulsive and the linear term is of opposite sign. H_R shares with H the property that its ground-state energy and wavefunction are exactly solvable and these in fact are still given by equations (2). However, arguments similar to those given above reveal that whereas the potential corresponding to H_R is confining for all non-zero values of λ, an infinitely wide oscillator well once again of depth $-\frac{1}{2}$ now develops in the limit $\lambda \to 0^+$, whereas at $\lambda = 0$ there is no confinement and hence there are only zero-energy bound states. Since the large-$|\lambda|$ behaviour of these eigenvalues are similar to those of H, we expect the energy spectrum to collapse to zero as $\lambda \to 0^-$ and when λ becomes positive we expect the levels to emerge from $-\frac{1}{2}$. This is borne out by Hill determinant calculations and we display the results in figure 2 which shows the anticipated behaviour of the eigenvalues of H_R as a function of λ. Once again the discontinuity at $\lambda = 0$ is evident.

Returning to the original Hamiltonian H, we notice that an obvious generalisation to consider is the Hamiltonian

$$\begin{aligned} H' &= p^2/2 - 1/r + 2\mu r + 2\lambda^2 r^2 \\ &= p^2/2 - 1/r - \mu^2/2\lambda^2 + 2(\lambda r + \mu/2\lambda)^2 \end{aligned} \tag{12}$$

which reduces to H for $\mu = \lambda$. We expect this system to display discontinuity in the eigenvalue spectrum only in the limit $\lambda \to 0$ and $\mu \to 0$ (see discussion at the end). If we further impose the condition that μ and λ go to this limit such that $\mu/\lambda = \text{constant} = \beta$, then the energy levels will collapse from the left into the value $-\beta^2/2$. For $\beta > 1$

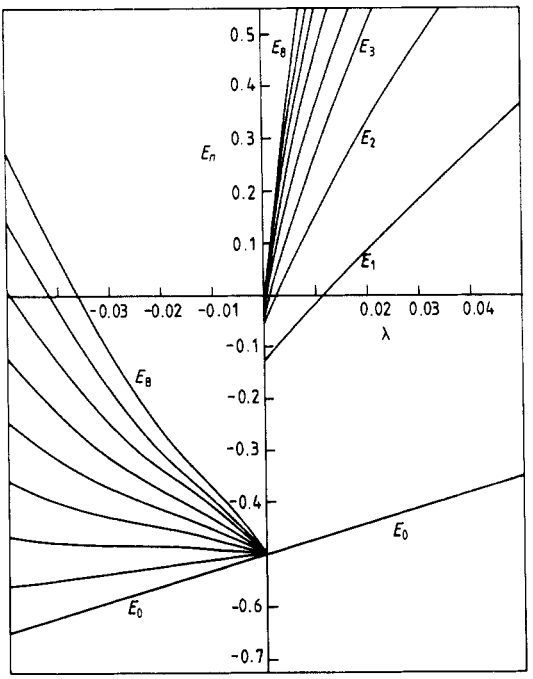

Figure 2. Plot of the first nine eigenvalues of the Hamiltonian (11) for $-0.1 \leqslant \lambda \leqslant 0.1$ calculated using the method of Hill determinants.

the accumulation point can be made lower than $-\frac{1}{2}$, the ground-state energy of the s-wave hydrogen atom. Starting with $\beta = 1$, if we make β tend to zero, the accumulation point of the energy levels can be gradually raised above $-\frac{1}{2}$ and as it rises above the Coulomb energy levels $-1/2(n+1)^2$, one by one these energy levels are expected to detach from the point of accumulation and become continuous with the Coulomb levels at $\mu = \lambda = 0$. We can therefore, by appropriate fine tuning, obtain an accumulation of energy levels wherever we want between 0 and $-\infty$. These conjectures are currently being investigated and the results will be published elsewhere.

It is worth contrasting here the situation in the present case with that for a classical system undergoing catastrophe. Consider a classical double-well potential in which the relative depth of the two minima is a function of a control parameter and the system to start with is located in the well with the lower minimum. If now the control parameter is varied so that the minimum of this well begins rising with respect to the other, the classical system makes a catastrophic transition to the other well at that value of the control parameter for which the well it was in is completely wiped out. In the corresponding quantum mechanical case, since the wavefunction of the system cannot be completely localised in either well alone, the question of a catastrophic transfer to the other well normally does not arise and no discontinuity is expected in the eigenvalue spectrum as a function of the control parameter. However, in the problem studied in this letter the system behaves much like a classical system, and we do see a discontinuity in the eigenvalue spectrum of the Hamiltonian H given by equation (1) because, as λ passes through zero from positive to negative, in addition to the Coulomb well at the origin a second well springs up suddenly as soon as λ becomes negative by an infinitesimal amount. A classical particle in this perturbation

potential if initially at the origin will continue to remain at the origin as λ goes from positive to negative since the Coulomb well at the origin persists for all values of λ. However, if we were to start with negative λ and the particle were located in the subsidiary well at $-1/2\lambda$, as λ approached 0^-, the particle would move away smoothly to infinity and then make a catastrophic jump to the origin as λ became positive and this subsidiary well was wiped out. A sudden change in the shape of the confining potential, like for example the sudden appearance of a well defined local minimum, appears therefore to be necessary for a quantum mechanical system to display discontinuity in its eigenvalue spectrum. Thus in the case of the Hamiltonian H' given by equation (12) it is necessary that both μ and λ vanish simultaneously in order to see a discontinuity in the eigenvalue spectrum. If λ is kept fixed at some non-zero value and μ is made to pass through zero from positive to negative, no discontinuity in the eigenvalue spectrum should be observed at $\mu = 0$ since now the second minimum at $r = -\mu/2\lambda^2$ would develop smoothly and not suddenly.

After this work was completed, we came across the paper by Calogero (1979) in which he discusses a class of Hamiltonians which have the property that their eigenvalue spectra show discontinuity at specific parameter values. Although the Killingbeck Hamiltonian (1) belongs to this class, it has the additional feature that, whereas all other eigenvalues are discontinuous across $\lambda = 0$, the ground-state energy remains continuous.

We conclude with the observation that, as more and more quantum mechanical systems are studied, the versatility and power of the method of Hill determinants for the numerical calculation of eigenvalues to arbitrary degree of accuracy become more and more evident. We know of no other method which could have allowed us to carry out the calculations reported in this letter with such a high degree of accuracy in a problem which is so sensitive to its parameters.

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