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LETTER TO THE EDITOR

Exact results for the potentials $V=-ax^{2s}+bx^{4s+2}$

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Abstract. The condition for a double-well potential $V=-ax^{2s}+bx^{4s+2}$ ($s=1,2,3,\ldots$) to have a negative energy branch is derived. For an arbitrary geometry of the well the total number of negative levels is determined. Some general features of the spectrum are pointed out. The results are based on a sequence of exactly obtainable zero energy solutions.

This work is based on the observation that for any member of the family of double well potentials

$$V=-ax^{2s}+bx^{4s+2} \tag{1}$$

with $a, b>0$ and s a positive integer, the single particle Schrödinger equation admits a sequence of zero energy solutions. In such cases the problem transforms into one of solving a two-term recursion relation whose admissible solutions require a suitable fine tuning of the coupling constants a and b. As a result one obtains a set of weighted polynomial solutions whose nodal characteristics determine the onset of the negative branch. One can, thereby, also determine the exact number of negative energy levels for arbitrary values of a, b and s. Some additional characteristics of the negative branch of the spectrum can also be deduced.

The Schrödinger equation of interest is

$$\Psi''+\left(\frac{2mE}{\hbar^2}+\frac{2ma}{\hbar^2}x^{2s}-\frac{2mb}{\hbar^2}x^{4s+2}\right)\Psi=0. \tag{2}$$

Primes denote derivatives with respect to x. Using dimensionless variables corresponding to the x^{2s} piece we can rewrite (2) as

$$\phi''+[\varepsilon+y^{2s}-\beta^2y^{4s+2}]\phi=0. \tag{3}$$

We have set $\Psi(x)\equiv\phi(y)$, $x=\alpha y$,

$$\alpha=\left(\frac{\hbar^2}{2ma}\right)^{1/(2s+2)} \qquad \beta^2=\frac{2mb}{\hbar^2}\alpha^{4s+4} \qquad \varepsilon=\frac{2mE}{\hbar^2}\alpha^2.$$

Letting

$$\phi=v\exp\left(-\frac{\beta y^{2s+2}}{2s+2}\right) \tag{4}$$

we find for the function $v(y)$, the equation

$$v''-2\beta y^{2s+1}v'+[\varepsilon+y^{2s}(1-\beta(2s+1))]v=0. \tag{5}$$

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For v, we introduce a power series expansion

$$v = \sum a_n x^n. \tag{6}$$

For even parity solutions $a_0 \neq 0$, $a_1 = 0$ and for odd parity solutions $a_0 = 0$, $a_1 \neq 0$. The coefficients $a_{-m} = 0$, $m = 1, 2, 3, \ldots$. Finally, we arrive at the three-term recursion relation

$$(n+2s+2)(n+2s+1)a_{n+2s+2} + \varepsilon a_{n+2s} + [1 - \beta(2n+2s+1)]a_n = 0. \tag{7}$$

Let us seek solutions of (7) with $\varepsilon = 0$. We thus have the problem of a two-term recursion relation, so that

$$a_{n+2s+2} = \frac{\beta(2n+2s+1)-1}{(n+2s+2)(n+2s+1)} a_n (\varepsilon = 0). \tag{8}$$

For arbitrary β the resulting solution is inadmissible since ϕ diverges as $\exp[\beta(y^{2s+2})/(2s+2)]$. But for

$$\beta = \frac{1}{2k+2s+1} \tag{9}$$

where

$$k = \begin{cases} p(2s+2) & \qquad (10a) \\ p(2s+2)+1 & \qquad p = 0, 1, 2 \ldots \qquad (10b) \end{cases}$$

the function v reduces to a polynomial of degree k. If (10a) holds, one has an even parity solution and if (10b) holds one has an odd parity solution. The coefficients in the expansion are given by

$$a_{n+2s+2} = \frac{2(n-k)}{(n+2s+2)(n+2s+1)(2k+2s+1)} a_n. \tag{11}$$

Thus, we have a manifestly normalizable $\varepsilon = 0$ solution for which v is a polynomial of degree k provided β is chosen as per (9) and k as per (10a) or (10b).

Let us consider the case $p = 0$. Then $k = 0$ or $k = 1$. For $k = 0$, $\varepsilon = 0$, $v =$ constant, ϕ is nodeless and $\beta = 1/(2s+1)$. It follows immediately that there can be no negative energy level for $\beta \geqslant 1/(2s+1)$. We are using an elementary quantum mechanical result that if $H \equiv H(g)$, $g \equiv \beta^2$, then $\partial\varepsilon/\partial g = \langle \partial H/\partial g \rangle$. In our case $\langle \partial H/\partial g \rangle$ is clearly positive. For $k = 1$, $\varepsilon = 0$, $v \sim x$, ϕ has one node and $\beta = 1/(2s+3)$. Hence, for $1/(2s+3) \leqslant \beta < 1/(2s+1)$ there is one and only one negative energy level. This is, of course, the ground state.

Next consider the $p = 1$ case. We have $k = 2s+2$ for the even solution and $k = 2s+3$ for the odd solution. These solutions have two and three nodes respectively and $\beta = 1/(6s+5)$ for the even case and $\beta = 1/(6s+7)$, for the odd case. Hence for $1/(6s+5) \leqslant \beta < 1/(2s+3)$ one has one pair of negative levels and for $1/(6s+7) \leqslant \beta < 1/(6s+5)$ there are three negative levels.

The wavefunctions for the $p = 1$ case are easily written down using (11). They have

$$v \sim (1 + ax^{2s+2}) \qquad \text{even}$$

$$v \sim x(1 + bx^{2s+2}) \qquad \text{odd.}$$

The coefficients a and b are given by (11).

Proceeding in this manner one easily finds that the number of negative levels is $(2p+1)$ as soon as k increases through the value given by (10a). There is no further increase until the k value passes that given by (10b). Here, we think of k as a continuous real variable that determines β through (9).

This completes the demonstration of our claim that the exact zero energy solutions that obtain for a discrete set of β values uniquely specify the number of negative levels for any β.

We now come to some other features of the spectrum suggested by this analysis.

It has been noted that a negative branch appears only if $\beta < 1/(2s+1)$. For $\beta = 1/(2s+1)$ the depth of the well is $((s+1)/(2s+1))[s(2s+1)]^{s/(s+1)}$. It follows that if $s \gg 1$, the well depth has to be larger than $\sim s^2$ for the onset of the negative branch. Hence, for large s the well has to be extremely deep for a negative level to appear. The coupling constant β^2 of the binding potential has to be vanishingly small for large s ($\beta^2 \ll 1/s^2$) for a negative branch to be realized.

It is amusing to note that for any double well of this family the special set of coupling constant values β^2 that give rise to the sequence of zero energy levels form a Rydberg-like progression.

Next, as k increases (s fixed) to values $\gg 1$, the special values of β given by (9) beyond which new negative levels appear form a quasi-discrete set. Hence, infinitesimal changes in β allow more and more levels to cross into the negative branch. But in such a case the geometry of the well changes very little. For example, there is only a small fractional change in the depth of the well as β moves to the next permissible value. Hence, qualitatively, one does not expect the levels that existed immediately below $\varepsilon = 0$ to move very much. It thus appears that the levels below $\varepsilon = 0$ and close to it form a converging pattern when followed from down to up towards $\varepsilon = 0$, for the case of deep wells ($k \gg 1$).

As a matter of fact, for the case of the sextic double-well potential discussed in [1] that corresponds to $s = 1$, such a convergence of levels is verifiable by a direct calculation. In this double-well case it is known that for $\beta = 1/(2k+3)$, the Hamiltonian develops an intimate connection with an underlying SL(2, R) symmetry [2]. Consequently, for $k = 2m$ or $k = 2m+1$, $m = 0, 1, 2, \ldots$, there appear $m+1$ exact solutions that correspond to the lowest lying $(m+1)$ levels of one parity. This set of $(m+1)$ levels can be deduced by elementary means (see [1] for details). One then finds that for $k \gg 1$, as we follow the levels of one parity from below towards $\varepsilon = 0$, they do indeed from a converging pattern. This convergence does not appear to be as pronounced as a Rydberg progression of levels. It may be remarked that a convergent pattern of levels for certain double wells has been suggested on the basis of supersymmetric quantum mechanics [3].

To conclude, it is worth stressing that one witnesses here a further utility of the subset of partial solutions that obtain for fine-tuned values of certain associated coupling constants. They have enabled us to deduce some spectral features of a whole class of potentials for the case of arbitrary couplings.

References

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