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Ouantum Harmonic Oscillators with Wave Functions Having a Fixed Logarithmic Derivative at the Equilibrium Position

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We construct the exact solution of the Schrödinger equation for the systems and the boundary condition stated in the title of this paper. The familiar cases of the ordinary harmonic oscillator and the half oscillator are immediately identified. The connection with the double oscillator is also established and is helpful to understand the energy spectrum of the latter. Similar connections can be used to study other partial oscillators.

Constroi-se a solução exata da equação de Schrödinger para os sistemas físicos e condições de contorno mencionados no título deste trabalho. Identificam-se imediatamente os casos familiares do oscilador harmônico comum e o meio oscilador. Também se estabelece a conexão com o oscilador duplo e espera-se entender o espectro de energia deste Último. Podem ser usadas conexões semelhantes para se estudar outros osciladores parciais.

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1. INTRODUCTION

In the most recent Latin American School of Physics, Wolf[1] discussed briefly the solution of the Schrödinger equation for the harmonic-oscillator potential with the boundary condition that the logarithmic derivative of the wave functions take a fixed value at the equilibrium position. The problem admits an exact solution and that discussion was in the context of noncompact group representations. We have studied the problem independently and here we present our version of the solution.

The formulation of the problem and the explicit construction of the solution, in both analytical and numerical forms, is presented in Section 2. In our discussion of Section 3, we identify immediately the familiar cases of the ordinary harmonic oscillator and the half oscillator, we establish the connection with the double oscillator and show its usefulness to understand the energy spectrum of the latter, and we illustrate how similar connection can be used to study other partial oscillators.

2. THE PROBLEM AND ITS SOLUTION

The Schrödinger equation for the harmonic oscillator of mass m, frequency ω and potential energy $m\omega^2x^2/2$, has the form

$$\left(-\frac{d^2}{dz^2}+\frac{z^2}{4}\right)\psi(z) = (\nu+\tfrac{1}{2})\psi(z) \quad , \tag{1}$$

in terms of the dimensionless coordinate $z=\sqrt{2m\omega/\hbar}\,x$ and the dimensionless energy parameter $\nu=(E/\hbar\omega)-\frac{1}{2}$. We are interested in constructing its wave functions such that i) they are quadradically integrable, for the time being in the interval $0\leqslant z<\infty$, which implies the boundary condition $\psi(z\to\infty)=0$, and ii) their logarithmic derivatives take a fixed value at the equilibrium position, say $\psi'(0)/\psi(0)=d$.

The boundary condition i) is common to the ordinary harmonic oscillator and the doubde oscillator[2], and we can make sure that it will be satisfied if we separate explícitly the usual Gaussian exponential factor in the wave function. Also, in common with these two cases, we can consider the two independent solutions $e^{-z^2/4}f$ and $e^{-z^2/4}zg$, whore remaining factors satisfy the respective equations obtained upon substitution in Eq. (1):

$$\xi \frac{d^2f}{d\xi^2} + (\tfrac{1}{2} - \xi) \frac{df}{d\xi} + \frac{\nu}{2} f = 0 \tag{2a}$$

$$\xi \frac{d^2g}{d\xi^2} + (\tfrac{3}{2} - \xi) \frac{dg}{d\xi} + \frac{\nu-1}{2} g = 0 \ . \tag{2b}$$

Here $\xi = z^2/2$, and both Eqs. (2a) and (2b) are immediately identified to be of the confluent hypergeometric type[3]. Then the general solution of Eq. (1) can be written as

$$\psi(z) = e^{-z^2/4} \left[A\,{}_1F_1(-\frac{\nu}{2};\frac{1}{2};\frac{z^2}{2}) + Bz\,{}_1F_1(\frac{1-\nu}{2};\frac{3}{2};\frac{z^2}{2})\right] \ . \tag{3a}$$

Now we proceed to analize how the boundary conditions can be implemented. From the asymptotic behavior of Kummer's confluent hypergeometric function ${}_1F_1(a;b;\xi\to\infty) \to \Gamma(b)e^{\xi}\,\xi^{a-b}/\Gamma(a)$, we see that the bracket in Eq. (3a) has the common factor $e^{z^2/2}$ which would dominate over the Gaussian exponential factor. Thus, boundary condition i) can be satisfied only if the remaining factor in the bracket vanishes, and this fixes the relative values of A and B leading to

$$\begin{aligned}\psi(z) &= ND_\nu(z)\\ &= N2^{\nu/2}\, e^{-z^2/4} \left[\frac{\Gamma(\frac{1}{2})}{\Gamma(\frac{1-\nu}{2})}\,{}_1F_1(-\frac{\nu}{2};\,\frac{1}{2};\,\frac{z^2}{z})\right.\\ &\qquad \left. + \frac{z^2}{\sqrt{2}}\,\frac{\Gamma(-\frac{1}{2})}{\Gamma(-\frac{\nu}{2})}\,{}_1F_1(\frac{1-\nu}{2};\,\frac{3}{2};\,\frac{z^2}{z})\right]\end{aligned} \tag{3b}$$

This is a parabolic cylinder function and is quoted directly in References (1) (2) and (3). The derivatives of this solution can be obtained, and making use of the properties of Kummer's function ${}_1F_1(a;b;0)=1$ and its derivative ${}_1F_1'(a;b;\xi) = (a/b)\,{}_1F_1(a+1;\ b+1;\xi)$, we can express the boundary condition ii) as

$$d = -\sqrt{2}\ \Gamma(\tfrac{1-\nu}{2})/\Gamma(-\tfrac{\nu}{2}) \tag{4}$$

This is a transcendental equation for the eigenvalues ν, which will take discrete values for a given logarithmic derivative. We carry out its numerical solution by assigning arbitrary values to ν and obtaining the corresponding values of d. A sample of them is given in Table I and in Figure 1. We find it convenient to use d or $1/d$ in a complementary way, depending on the situation.

We close this section by pointing out that we have constructed the solution of Eq. (1) subject to the boundary conditions i) and ii), obtaining the eigenvalues, Eq. (4), and the eigenfunctions, Eq. (3b). Concerning the latter, it is straightforward to show that they also satisfy the orthogonality condition, as expected from Sturm--Liouville theory[4].

3. DISCUSSION

From Table I and Fig. 1 we immediately recognize the equally spaced energy spectrum of the ordinary harmonic oscillator[2], $-\infty < z < \infty$, which corresponds to the integer values of $\nu = 0,1,2,3,4,5,\ldots,$ associated alternately with vanishing values of d and $1/d$. Of course, only either of these two conditions can provide a smooth matching of our results in the interval $0 \leq z < \infty$ to those of the system under consideration. In fact, they can be identified as the even and odd parity states, which have a derivative of the wave function and a wave function, respectively, vanishing at $z=0$. Equation (4) is clearly satisfied in both cases, and Eq. (3b) shows that the wave function is reduced to only the first term and to only the second term, in the respective cases. Additionally, the corresponding Kummer functions, having a negative integer as their first parameter, become polynomials

TABLE I - Eigenvalues and Logarithmic Derivatives at the Equilibrium Position for Harmonic Oscillators.

ν	d	$1/d$
-0.8	-0.681317	-1.467746
-0.6	-0.550370	-1.816960
-0.4	-0.399867	-2.500831
-0.2	-0.221373	-4.517258
0.0	0.000000	∞
0.2	0.293549	3.406584
0.4	0.726784	1.375925
0.6	1.500498	0.666445
0.8	3.613807	0.276717
1.0	∞	0.000000
1.2	-4.087900	-0.244624
1.4	-1.926295	-0.519131
1.6	-1.066312	-0.937811
1.8	-0.498090	-2.007670
2.0	0.000000	∞
2.2	0.538173	1.858137
2.4	1.245915	0.802623
2.6	2.438310	0.410120
2.8	5.621477	0.177889
3.0	∞	0.000000
3.2	-5.946037	-0.168179
3.4	-2.728917	-0.366446
3.6	-1.476432	-0.677308
3.8	-0.675979	-1.479336
4.0	0.000000	∞
4.2	0.706352	1.415723
4.4	1.612361	0.620209
4.6	3.115618	0.320963
4.8	7.100813	0.140828
5.0	∞	0.000000

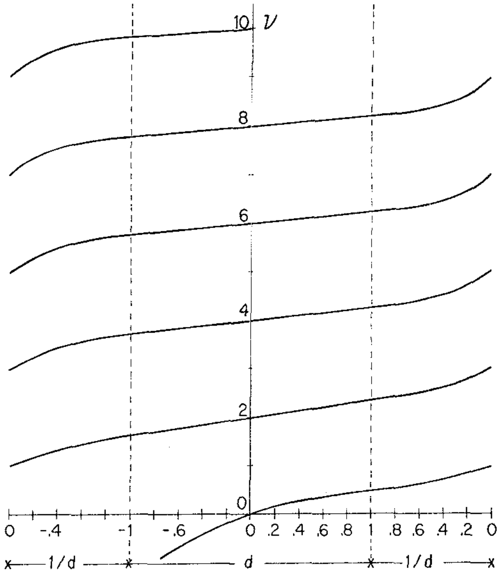

Fig.1 - Energy spectra for harmonic oscillators whose wave functions have a fixed logarithmic derivative at the equilibrium position.

and their identification with the Hermite polynomials is also immediate.

The half oscillator[5], defined by the harmonic oscillator potential in the interval $0 < z < \infty$ and an infinitely high potential barrier for $z<0$, has the boundary condition of a vanishing wave function at $z=0$, i.e. $1/d = 0$. In this case, Table I shows that the energy spectrum is also equally spaced, but with a spacing double that of the ordinary harmonic oscillator, because ν is restricted now to only odd integer values. Correspondingly the wave functions belong to the odd parity set of the ordinary harmonic oscillator. In Fig. 1, these states appear at either extreme end.

These two familiar cases, involving vanishing values of d and $1/d$, are incidentally the only cases of equally spaced energy levels. Tabie I and Fig. 1 show that for other values of d and $1/d$ the energy levels are indeed unequally spaced. However, apart from this, the corresponding states do have in common with the ordinary harmonic oscillator states some other general properties. Among them we already mentioned that of orthogonality. By making reference to' Fig. 1, we can say thqt the lowest branch corresponds to the ground states for the different values of d; they all have in common wave functions without any zeros in the interval $0 \leq z < \infty$. The successive branches above correspond to the first, second, third,... excited states; their respective wave functions have one, two, three, ... zeros in the interval $0 \leq z < \infty$. Furthermore, for each branch we can distinguish the left (L, $d<0$) and the right (R, $d \geq 0$) halves; their corresponding wave functions have a number of maxima and minirna equal to their number of zeros andtotheir number of zeros plus one, respectively. If we adopttheconvention that the wave functions approach zero asyrnptotically from above, i.e. with a positive value, then the number of maxima is equal to the number of minima arid to the number of minima plus one, in the left right halves of a brarich, respectively. This type of information about the wave functions is summarized in Table II, and illustrated in Fig. 2. For a given branch, characterized by the number of zeros in the wave functions, the larger the value of d the farther out are the positions of the corresponding zeros, $z_{oi}^{(n)}$, maxima, $z_{Mj}^{(n)}$, and rninima, $z_{mk}^{(n)}$, of the respective wave functions, i.e. if $d_1 < d_2$, then

$$z_{oi}^{(n)}(d_1) < z_{oi}^{(n)}(d_2) \tag{5a}$$

$$z_{Mj}^{(n)}(d_1) < z_{Mj}^{(n)}(d_2) \tag{5b}$$

$$z_{mk}^{(n)}(d_1) < z_{mk}^{(n)}(d_2) \tag{5c}$$

where $i = 1,2,\ldots,n$; $j = 1,2,\ldots n$; $k = 1,2,\ldots$ distinguish the ordered points of each kind. On the other hand, for a given value of d, the zeros of the wave functions of the different eigenstates are related to each other through

$$\begin{gathered} z_{01}^{(1)} < z_{02}^{(2)} < z_{03}^{(3)} < \ldots < z_{0n}^{(n)} < z_{0n+1}^{(n+1)} < \ldots , \\ z_{01}^{(2)} < z_{02}^{(3)} < \ldots < z_{0\,n-1}^{(n)} < z_{0\,n}^{(n+1)} < \ldots , \\ \ldots \\ z_{0i}^{(n)} < z_{0i+1}^{(n+1)} < \ldots \end{gathered} \tag{6}$$

TABLE II - Characteristics of Wave Functions for Harmonic Oscillators in the Interval $0 \leqslant z < \infty$ for different Eigenvalues and Logarithmic Derivatives at the Equilibrium Position. The symbol $[\ ]$ indicates that we take only the integer part of the number inside.

ν	d	Number of Zeros	Numbers of Maxima and Minima
$(-\infty,0)$	$(-\infty,0)$	0	$0 = 0 + 0$
$[0,1)$	$[0,\infty)$	0	$1 = 1 + 0$
$[1,2$	$(-\infty,0)$	1	$1 = 1 + 0$
$[2,3)$	$[0,\infty)$	1	$2 = 1 + 1$
$[3,4)$	$[-\infty,0)$	2	$2 = 1 + 1$
$[4,5)$	$[0,\infty)$	2	$3 = 2 + 1$
$[5,6)$	$[-\infty,0)$	3	$3 = 2 + 1$
$[6,7)$	$[0,\infty)$	3	$4 = 2 + 2$
...	...	...	...
$[2n-1,2n)$	$(-\infty,0)$	n	$n = \left[\frac{n+1}{2}\right] + \left[\frac{n}{2}\right]$
$[2n,2n+1)$	$[0,\infty)$	n	$n+1 = \left[\frac{n+2}{2}\right] + \left[\frac{n+1}{2}\right]$

Similar inequalities hold for their maxima and their minima. Thus, for half branches on the left,

$$z_{M1}^{(1)} < z_{M1}^{(2)} < z_{M2}^{(3)} < z_{M2}^{(4)} < \dots z_{M[(n+1)/2]}^{(n)} < z_{M[(n+2)/2]}^{(n+1)} < \dots , \quad (7a)$$

$$z_{m1}^{(2)} < z_{m1}^{(3)} < z_{m2}^{(4)} < z_{m2}^{(5)} < \dots \quad z_{m[n/2]}^{(n)} < z_{m[(n+1)/2]}^{(n+1)} < \dots ; \quad (7b)$$

while for half branches on the right,

$$z_{M1}^{(0)} < z_{M1}^{(1)} < z_{M2}^{(2)} < z_{M2}^{(3)} < \dots < z_{M[(n+2)/2]}^{(n)} < z_{M[(n+3)/2]}^{(n+1)} < \dots , \quad (7c)$$

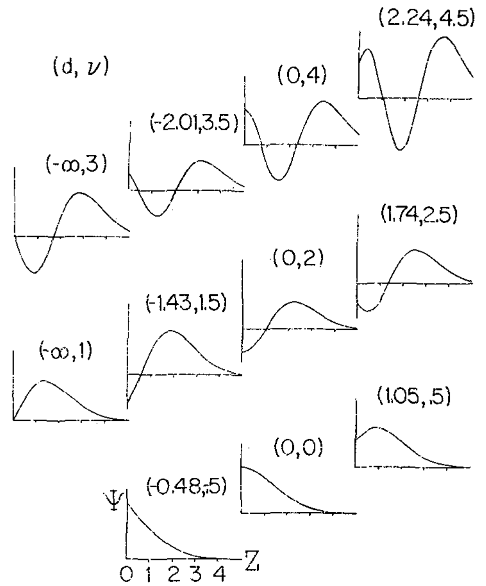

Fig.2 - Wave functions for harmonic oscillators with different logarithmic derivatives at the equilibrium position and energies.

$$z_{m1}^{(1)} < z_{m1}^{(2)} < z_{m2}^{(3)} < z_{m2}^{(4)} < \dots < z_{m[(n+1)/2]}^{(n)} < z_{m[(n+2)/2]}^{(n+1)} < \dots . \qquad (7d)$$

We will make use of some of the above properties to discuss qualitatively the less-than-half, the more-than-half and the double oscillators.

In analogy with the half oscillator, the less-than-half oscillator is defined by the harmonic oscillator potential in the interval $c < z < \infty$ and an infinitely high potential barrier for $z<c$. Consequently, its wave functions are also given by Eq. (3b), which satisfies i), and must also satisfy the boundary condition ii) $\psi(z=c) = 0$. The latter implies that the zeros of Eq. (3b) must coincide with c,

$$z_{0i}^{(n)}(d) = c , \qquad (8a)$$

and they determine the eigenstates of the system. From Fig. 2, it is clear that there is no solution for $n = 0$, i.e. $\nu < 1$. Actually, for a given value of c, the ground state of the system will have its energy in the interval $1 < \nu < 3$, corresponding to

$$z_{01}^{(1)}(d) = c \ ; \tag{8b}$$

or in the interval $3 < \nu < 5$, corresponding to

$$z_{02}^{(2)}(d) = c \ ; \tag{8c}$$

or, in general, in the interval $2n-1 < \nu < 2n+1$ corresponding to

$$z_{0n}^{(n)}(d) = c \ . \tag{8d}$$

Similarly, the first excited state must have $\nu > 3$, and its position will be in the interval $3 < \nu < 5$, $5 < \nu < 7, \ldots, 2n-1 < \nu < 2n+1$ depending on the existence of the solution of

$$z_{01}^{(2)}(d) = c \ , \quad z_{02}^{(3)}(d) = c \ , \ldots \quad z_{0\,n-1}^{(n)}(d) = c \ . \tag{8e}$$

In general, the ℓ-th excited state must have $\nu > 2\ell+1$, and its position will be in the interval $2n-1 < \nu < 2n+1$ where a solution of

$$z_{0\,n-\ell}^{(n)}(d) = c \tag{8f}$$

exists. The interlacing of the zeros, Ineqs. (5a) and (6), combined with Eq. (4), guarantee that the solution of Eq. (8f) is unique for a fixed value of c. On the other hand, we could construct globally the energy spectra of less-than-half oscillators with varying values of c, by extracting the values of $c = z_{0i}^{(n)}$ and ν from a source analogous to Fig. 2 and making the necessary interpolating. The corresponding $(c, \nu^{(\ell)})$ curves are monotonically increasing lines starting from $(c=0, \nu^{(\ell)} = 2\ell+1)$.

The more-than-half oscillator is defined by the harmonic oscillator potential in the interval $-c < z < \infty$ and an infinitely high potential barrier for $z < -c$. Again, its wave functions are also given by Eq. (3b), satisfy i), and must also satisfy the boundary condition ii)'' $\psi(z=-c) = 0$. Let us recall that Eq. (3b) was constructed with the interval $0 \leq z < \infty$ in mind, but it can be extrapolated to $-c < z < 0$ without any difficulty. It must be pointed out that for d or 1/d different from zero, the wave function in Eq. (3b) is divergent approaching $+\infty$ and $-\infty$ for left and right half branches, respectively, as $z \to -\infty$; ttowever, this need not bother us for, finite values of c, where the interval of extrapolation is also finite. In such an extrapolation, the even and odd parity terms will dominate when $d = 0$ and $1/d \approx 0$, respectively; naturally, the extreme cases of exact equality correspond to the situations dealt with in the first paragraph of this section. The number of zeros of the wave functions in the interval $-\infty \leqslant z < 0$ is equal to n for the left half branches and to n+l for the right half branches. From our knowledge of the ground state wave functions for the ordinary harmonic oscillator (d=0, ν=0) and the half oscillator (d=-∞, ν=1), we know that they cannot satisfy i , except for $c \to \infty$. For a finite value of c, the ground state of the more-than -half oscillator corresponds to some point in the right half of the n=O branch of Figs. 1 and 2 (d>0, 0<ν<1), where the wave functions have the right value of d to be able to satisfy ii)" upon extrapolation; the smaller the value of c the larger has to be the value of d and viceversa. Thus, starting from c=0, we have the half-oscillator with ν=1; as c increases, ν decreases monotonically; and their asymptotic values ∞ and 0 correspond to the ordinary complete oscillator. The wave function of the first excited state of the more-than-half oscillator is characterized by having one zero in the interval $-c<z<\infty$; such a condition can be satisfied by wave functions associated with the branch of Figs. 1 arid 2 in the intervals $1<\nu<3$ and $\infty>c>0$ giving again a monotonic decrease of the energy from that of the half oscillator (c=0, ν=3) to that of the complete oscillator (c=∞, ν=1). Similarly, the wave function of the second excited state is characterized by having two zeros in the interval $-c<z<\infty$, and Figs. 1 and 2 help us to recognize that this can be accomplished within the intervals $2<\nu<5$ and $\infty>c>0$; this gives the monotonic decrease of the energy from the half oscillator (c=0, ν=5) to the complete oscillator (c=∞, ν=2). The generalization follows immediately: the global energy spectra for more-than-half oscillators with different values of c concist of monotonically decreasing lines starting from the half oscillator (c=0, $\nu^{(\ell)}=2\ell+1$) and going down to the complete oscillator (c=∞, $\nu^{(\ell)}=\ell$). Such lines can be identified in Fig. 5.4 of Ref.2, where they appear as part of the spectra of the double oscillator. Also, these energy lines are smoothly connected with those of the less-than-half oscillators. Actually all these partial oscillators could be treated in a unified way by allowing c to be positive or negative in ii)'.

The double oscillator is defined by the harmonic oscillator potential centered at $y = c$, for $0 < y < \infty$, and at $y = -c$, for $-\infty < y < 0$. The system is symmetric under the reflection operation $y \rightarrow -y$, and therefore its wave functions have a well defined parity. The connection between the double oscillator and our problem is established by shifting the origin so that $z = y - r$ and making the reflection with respect to $y=0$. Then the boundary conditions for the odd and even parity states are ii)'' $\psi(y=0) = \psi(z=-c) = 0$ and ii)''' $\psi'(y=0) = \psi'(z=-c) = 0$, respectively. We see that ii)'' is the condition that we already investigated for the more-than-half oscillators, and consequently those results are identified as corresponding to the odd-parity states of the double oscillator. The boundary condition ii)''' involves the maxima or minima of our problem in the extrapolated interval $-\infty < z < 0$. The number of maxima and minima of the wave functions in the interval $-\infty < z < 0$. The number of maxima and minima of the wave functions in the interval $z_{OE} < z < 0$, where z_{OE} is the zero in the extreme left, is equal to n for both the left and the right halves of a branch; for $-\infty < z < a_{OE}$, there are none at the Deginning of a half branch, and there are additionally one maximum and one minimum at the end of each half branch. Starting from the extreme end of a half branch these points can be identified with the point at $z = -\infty$ and the maximum or minimum at the extreme left of the corresponding wave functions for the ordinary harmonic oscillator; as we move down along the half branch, such points will move towards each other, until they coalesce into an inflection point $z_{ME} = z_{mE} = z_{IE} < z_{OE}$ and then they dissappear. This information is useful to describe the variation of the even parity energy levels of the double oscillator as the value of c changes. In fact, for the ground state and starting with $c=0$, we have the ordinary harmonic oscillator ground state ($d=0$, $\nu=0$); a5 c increases we have to move down along the lowest left half branch ($d<0$, $\nu<0$) in order to be able to satisfy ii)'''. For small values of c this can be satisfied if the extrapolated wave function has its maximum at the right position $z_{MF}^{(OL)}(d) = -c$; thus, ν decreases as c increases from zero up to $c = -z_{IE}^{(OL)}$. From here on, as c increases more, we have to moveupalong the lowest half branch and ii)''' is satisfied at the minimum of the extrapolated wave function $z_{mE}^{(OL)}(d) = -c$; as $c \to \infty$, we come back asymptotically and from below to the ordinary harmonic oscillator ground state. Similarly, the first excited even parity state of the double oscillator starts from the corresponding state of the ordinary harmonic oscillator (d=0, ν=2) for c=0; its energy decreases monotonically, as c increases, covering the interval $2<\nu<1$, where $z_{mE}^{(1L)}(d) = -c$ and the interval $1<\nu<\nu_{IE}^{(OR)}$, where $z_{ME}^{(OR)}(d) = -c$ up to $z_{IE}^{(OR)} = -c$; and from here on, the energy increases covering the interval $\nu_{IE}^{(OR)} < \nu < 1$, where $z_{mE}^{(OR)}(d) = -c$, approaching asymptotically and from below the first excited energy level of the ordinary harmonic oscillator ($1/d$=0, ν=1) for $c\to\infty$. In general, the global energy levels for the even parity states of the double oscillator consist of lines which start from the corresponding states of the ordinary harmonic oscillator (c=0, $\nu=2\ell$); decrease monotonically down to ($c = -z_{IE}$, $\nu = \nu_{IE} < \ell$), where they are minima; and then increase in the intervals ($-z_{IE} < c < \infty$, $\nu_{IE} < \nu < \ell$) approaching asymptotically and from below the $\nu=\ell$ state of the ordinary harmonic oscillator for $c \to \infty$. The two lowest even parity energy levels of the double oscillator also appear in Fig. 5.4 of Ref. 2. The pairing of consecutive even and odd parity energy levels, which approach asymptotically the ordinary harmonic oscillator energy levels from below end above, respectively, is also established. The discussion in this section has been intentionally qualitative in order to give an overall understanding of the energy spectra and wave functions of the different oscillators considered, as well as the connections among them. On the other hand, the quantitative formulation of Section 2, Eq. (3b), contains the elements to construct the numerical solutions for specific situations.

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description of free electrons near the surface of a solid under a uniform magnetic field.[6]

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