

EXPONENTIALLY CONFINING POTENTIAL WELL

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We introduce an exponentially confining potential well that can be used as a model to describe the structure of a strongly localized system. We obtain an approximate partial solution of the Schrödinger equation with this potential well where we find the lowest energy spectrum and the corresponding wavefunctions. We use the tridiagonal representation approach as the method for obtaining the solution as a finite series of square-integrable functions written in terms of Bessel polynomials.

Keywords: exponential potential, tridiagonal representation approach, Bessel polynomial

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*To the memory of my friend, colleague, and collaborator,
the late Mohammed S. Abdelmonem*

1. Introduction

Confining potentials are used as models to describe the structure of bound systems with strong localization. The harmonic oscillator potential, which is treated in most textbooks on quantum mechanics, is the most popular (see, e.g., [1]). Other models include the linear potential, which is sometimes used to describe the confinement of quarks inside hadrons [2], [3]. These two models respectively describe confinement of a quadratic and linear strength. In addition to the infinite square well and the quartic potentials, there is rarely any treatment in the literature of potentials with extreme confinement strength including those of the exponential type. If there is interest in models with extreme confinement but without infinitely hard boundaries (to allow for some level of wall penetration and nonvanishing of the wave function tail into the walls), then the infinite square well potential cannot be used, and a confinement with greater than power-law strength is needed.

Here, we provide a one-dimensional model over the whole real line with a confinement strength that grows exponentially. Specifically, we propose the potential model

$$V(x) = \frac{\lambda^2}{2} \left(\frac{1}{4} e^{-2\lambda x} - A_- e^{-\lambda x} + A_+ e^{\lambda x} \right), \quad (1)$$

where $-\infty < x < +\infty$ and we use the atomic units $\hbar = M = 1$. The scale parameter λ is real with the dimension inverse length, which is a measure of the range of the potential. The parameters A_{\pm} are real and dimensionless with $A_+ > 0$. We plot this potential in Fig. 1 for a fixed A_+ and several values of A_- . Changing the sign of λ causes a reflection of the plot with respect to the vertical axis. Zooming out along the vertical axis in the figure (i.e., for large energies), the potential mimics an infinite square well.

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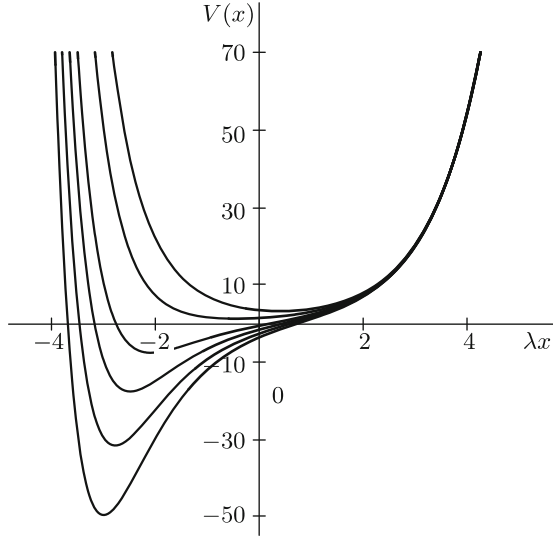


Fig. 1. Potential (1) for $\lambda = 1$, $A_+ = 2$, and several values of A_- : the six curves from the top down correspond to $A_- = -4, 0, 4, 6, 8, 10$.

The Schrödinger equation with potential function (1) is not exactly solvable using any of the conventional solution methods unless $A_+ = 0$, in which case (1) becomes the Morse potential. Such conventional methods include factorizations, a point canonical transformation, supersymmetry, shape invariance, the Darboux transformation, second quantization, the asymptotic iteration method, group theory, the path integral transformation, the Nikiforov–Uvarov method, etc. (see, e.g., [4]–[11] for a description of these methods). Nevertheless, we here show that the newly introduced algebraic solution method called the tridiagonal representation approach (TRA) [12] yields a quasi-exact solution of this problem in the form of a bounded series of square-integrable functions. The expansion coefficients of the series are orthogonal polynomials in the energy and physical parameter space.

We start by writing the solution of the Schrödinger equation with potential (1) as the series

$$\psi(x) = \sum_n f_n \phi_n(x), \quad (2)$$

where $\{\phi_n(x)\}$ is a complete set of square-integrable functions that vanish at infinity and $\{f_n\}$ are the expansion coefficients. After a coordinate transformation to the dimensionless variable $y(x) = e^{\lambda x}$, the resulting time-independent Schrödinger equation suggests that we choose the basis set with the elements

$$\phi_n(x) = G_n y^\alpha e^{-\beta/y} J_n^\mu(y), \quad (3)$$

where $J_n^\mu(y)$ is the Bessel polynomial whose properties are given in Appendix A. The parameter μ is negative such that $\mu < -N - 1/2$, where N is a nonnegative integer and $n = 0, 1, \dots, N$. The dimensionless real parameters α and β are determined below, and the normalization constant is conveniently chosen as $G_n = \sqrt{-(2n + 2\mu + 1)/(n! \Gamma(-n - 2\mu))}$.

Our choice of a basis of form (3) is suggested by the TRA requirement. We could not find an alternative basis set that results in a tridiagonal matrix representation for the wave operator with potential (1). Unfortunately, this basis set is incomplete. Physically, completeness of a *discrete* basis set means that, first, its size is infinite; second, it is defined over the whole configuration space of the physical problem; third, it satisfies the boundary conditions. The last requirement usually implies that the basis elements are square

integrable. Rigorously, we should also require that the basis set be dense over the whole configuration space. For example, deleting some finite subset of the infinite basis makes it incomplete. On the other hand, a finite basis set can in fact give a faithful physical representation of the system if the system has a finite spectrum and the size of the basis is not less than the size of the spectrum. We confirm this observation below in the case of potential (1) with $A_+ = 0$, where it becomes the Morse potential with a finite spectrum.

Therefore, we must conclude that we can use a finite basis set to give an approximate representation of a physical system with an infinite spectrum like potential (1) and that the approximation improves as the size of the basis increases. Below, we unfortunately find that the size of our basis set is constrained by physical requirements and cannot be arbitrarily increased. On the other hand, it might be possible that a finite basis set gives an exact representation for a part of the infinite spectrum whose size does not exceed the size of the basis set. Such a solution is said to be quasi-exact. By definition, a quasi-exact solution is a partial exact solution where part (not all) of the energy spectrum is obtained (see, e.g., [13]). If the size of the basis is equal to the size of the quasi-exact solutions, then the representation is diagonal and not tridiagonal, i.e., the basis elements are in fact the eigenvectors of the associated Hamiltonian in the finite quasi-exact subspace.

In the atomic units, the time-independent Schrödinger equation for potential (1) is written in terms of the dimensionless variable y as

$$\left[y^2 \frac{d^2}{dy^2} + y \frac{d}{dy} - U(y) + \varepsilon \right] \psi(y) = 0, \quad (4)$$

where

$$U(y) = \frac{2V(x)}{\lambda^2} = \frac{1}{4y^2} - \frac{1}{y}A_- + A_+y, \quad \varepsilon = \frac{2E}{\lambda^2}.$$

If we write this wave equation as $\hat{J}\psi(y) = 0$ and substitute ansatz (2), then finding the solution requires evaluating the action of the wave operator on the basis elements, $\hat{J}\phi_n(y)$. The TRA dictates that this action must have the tridiagonal structure [12]

$$\hat{J}\phi_n(y) = \omega(y)[c_n\phi_n(y) + b_{n-1}\phi_{n-1}(y) + b_n\phi_{n+1}(y)], \quad (5)$$

where $\omega(y)$ is a nonzero analytic function on the whole real line and the coefficients c_n and b_n are y -independent and such that $b_n^2 > 0$ for all n .

Substituting (2) into (4) and using (5), we convert the problem into finding a solution of the discrete algebraic equation

$$zP_n = a_nP_n + b_{n-1}P_{n-1} + b_nP_{n+1}, \quad (6)$$

where $c_n = a_n - z$ and $f_n = f_0P_n$ and hence $P_0 = 1$. Equation (6) is a three-term recurrence relation whose solution (because $b_n^2 > 0$) is an orthogonal polynomial in z if we require that the expansion coefficients a_n and b_n be independent of z [14], [15].

It turns out that the polynomial argument z depends on the energy and/or physical parameters of the problem. It was previously shown that all physical properties of the system (the energy spectrum of bound states, the shift of the scattering phase, the density of states, etc.) can be obtained from the properties of the orthogonal polynomial $P_n(z)$ (its weight and generating functions, structure of zeros, asymptotic behavior, etc.) [12], [16], [17]. It was also shown that the positive-definite weight function of $P_n(z)$ is equal to $f_0^2(z)$.

In the next section, we use the TRA tools to obtain recurrence relation (6) associated with potential function (1) and attempt to find the corresponding orthogonal polynomial $P_n(z)$, whence we obtain the physical properties of the system.

2. The TRA solution

Using basis elements (3), after several differential manipulations, we obtain

$$\hat{J}\phi_n(y) = G_n y^\alpha e^{-\beta/y} \left\{ y^2 \frac{d^2}{dy^2} + [y(2\alpha + 1) + 2\beta] \frac{d}{dy} + \frac{1}{y} \beta(2\alpha - 1) + \frac{\beta^2}{y^2} + \alpha^2 - U(y) + \varepsilon \right\} J_n^\mu(y). \quad (7)$$

Applying the differential equation of the Jacobi polynomial (see Eq. (A.4) in Appendix A), we bring this equation to the form

$$\begin{aligned} \hat{J}\phi_n(y) = G_n y^\alpha e^{-\beta/y} \left\{ \left[2y \left(\alpha - \mu - \frac{1}{2} \right) + 2\beta - 1 \right] \frac{d}{dy} + \frac{1}{y} \beta(2\alpha - 1) + \right. \\ \left. + \frac{\beta^2}{y^2} + \alpha^2 - U(y) + n(n + 2\mu + 1) + \varepsilon \right\} J_n^\mu(y). \end{aligned} \quad (8)$$

Choosing $\alpha = \mu + 1/2$ and $\beta = 1/2$ as the basis parameters, we eliminate the derivative term and bring this equation to the simple form

$$\hat{J}\phi_n(y) = G_n y^{\mu+1/2} e^{-1/2y} \left[\frac{\mu}{y} + \frac{1}{4y^2} + \left(n + \mu + \frac{1}{2} \right)^2 - U(y) + \varepsilon \right] J_n^\mu(y). \quad (9)$$

The compatibility of TRA conditions (5) and the properties of the Bessel polynomial in Appendix A now means that the expression in the square brackets must be a linear function of y . Terms that are not linear must be eliminated by counterterms in $U(y)$. Therefore, the most general form of $U(y)$ preserving the tridiagonal structure of (5) is

$$U(y) = \frac{1}{4y^2} + \frac{U_0}{y} + U_1 y, \quad (10)$$

in which case we choose the basis parameter $\mu = U_0$ and U_1 is an arbitrary real parameter. In fact, this is exactly potential (1) presented above with $U_0 = -A_-$ and $U_1 = A_+$. We note that any constant in the potential function $U(y)$ can be absorbed into the energy ε by a simple redefinition.

With the above form of $U(y)$, Eq. (9) becomes

$$\hat{J}\phi_n(x) = G_n y^{\mu+1/2} e^{-1/2y} \left[-A_+ y + \left(n + \mu + \frac{1}{2} \right)^2 + \varepsilon \right] J_n^\mu(y), \quad (11)$$

where $\mu = -A_-$. The first term $-A_+ y$ is evaluated using the recurrence relation (A.2) in Appendix A, and we obtain

$$\begin{aligned} \hat{J}\phi_n(x) = \omega(x) \left\{ \left[\frac{-2\mu}{(n+\mu)(n+\mu+1)} - \frac{4}{A_+} \left(n + \mu + \frac{1}{2} \right)^2 - \frac{4\varepsilon}{A_+} \right] \phi_n(x) - \right. \\ \left. - \frac{n}{(n+\mu)(n+\mu+1/2)} \frac{G_n}{G_{n-1}} \phi_{n-1}(x) + \frac{n+2\mu+1}{(n+\mu+1)(n+\mu+1/2)} \frac{G_n}{G_{n+1}} \phi_{n+1}(x) \right\}, \end{aligned} \quad (12)$$

where $\omega(x) = -A_+/4$. This equation coincides with (5) if we set

$$c_n = \frac{-2\mu}{(n+\mu)(n+\mu+1)} - \frac{4}{A_+} \left(n + \mu + \frac{1}{2} \right)^2 - \frac{4\varepsilon}{A_+}, \quad (13)$$

$$b_n = -\frac{1}{n+\mu+1} \sqrt{\frac{-(n+1)(n+2\mu+1)}{(n+\mu+1/2)(n+\mu+3/2)}}. \quad (14)$$

We note that because the range of μ is bounded by the inequality $\mu < -N - 1/2$, the radicand in (14) is always positive, which gives $b_n^2 > 0$ for $n = 0, 1, \dots, N - 1$. If $c_n = a_n - z = a_n - 4\varepsilon/A_+$, then we obtain three-term recurrence relation (6) for the polynomial $P_n(4\varepsilon/A_+)$. To find this orthogonal polynomial, which contains all physical properties of the system, we first bring the recurrence relation to a standard form. We define the polynomial $B_n^\mu(z; \gamma)$ by the equality $P_n(z) = (G_n/G_0)B_n^\mu(z; \gamma)$, where $\gamma = -4/A_+$ and the normalization constant G_n is given below Eq. (3). As a result, we have the recurrence relation for $B_n^\mu(z; \gamma)$

$$zB_n^\mu(z; \gamma) = \left[\frac{-2\mu}{(n+\mu)(n+\mu+1)} + \gamma \left(n + \mu + \frac{1}{2} \right)^2 \right] B_n^\mu(z; \gamma) - \frac{n}{(n+\mu)(n+\mu+1/2)} B_{n-1}^\mu(z; \gamma) + \frac{n+2\mu+1}{(n+\mu+1)(n+\mu+1/2)} B_{n+1}^\mu(z; \gamma). \quad (15)$$

Using it with $B_{-1}^\mu(z; \gamma) = 0$ and $B_0^\mu(z; \gamma) = 1$, we obtain the explicit form of all polynomials $B_n^\mu(z; \gamma)$ for $n = 0, 1, \dots, N - 1$. We note that (15) differs significantly from relation (A.2) for the Bessel polynomials because the term $(n + \mu + 1/2)^2$ is present in the diagonal term of the recursion. But if we choose $\gamma = 0$, then we have $B_n^\mu(z; 0) = J_n^\mu(z/4)$.

All our attempts to match $B_n^\mu(z; \gamma)$ with known polynomials failed. We tried using the table of recurrence relations in [14] and the properties of the hypergeometric orthogonal polynomials in [18]. We also looked at the chapter on orthogonal polynomials in the *Digital Library of Mathematical Functions* [19] and compared with the information available in *CAOP - Computer Algebra & Orthogonal Polynomials* [20]. Moreover, we tried using computer algebra systems (such as `rec2ortho` or `retode` [21]), where polynomials can be obtained from their recurrence relations. Consequently, we were forced to resort to numerical analysis to extract the physical information from $B_n^\mu(z; \gamma)$; we present the results in Sec. 3.

The solution of the Schrödinger equation with potential (1) as a partial sum has the form

$$\psi(x) = \sqrt{\rho \left(\frac{4\varepsilon}{A_+} \right)} \sum_{n=0}^{N-1} B_n^\mu \left(\frac{4}{A_+}; -\frac{4\varepsilon}{A_+} \right) \phi_n(x), \quad (16)$$

where the basis functions $\phi_n(x)$ are given by (3) with $\mu = -A_-$, $\alpha = \mu + 1/2$, and $\beta = 1/2$. The function $\rho(z)$ is the positive-definite weight function for the polynomial $B_n^\mu(z; \gamma)$. We note that it follows from the condition $\mu < -N - 1/2$ that the number of bound states N obtained by the TRA is the largest integer not exceeding $A_- - 1/2$. But the actual number of bound states associated with this confining potential is obviously infinite. Therefore, our solution of the problem obtained using the TRA is (at best) quasi-exact. In the next section, we calculate the lowest bound state energies and construct the corresponding wave functions.

3. Results and discussion

The first direct and almost trivial result occurs for $A_+ = 0$. As can be seen from Eq. (11), in this case, we obtain a diagonal (not tridiagonal) representation, and the energy spectrum becomes $\varepsilon_n = -(n + \mu + 1/2)^2$, in other words,

$$E_n = -\frac{1}{2}\lambda^2 \left(n - A_- + \frac{1}{2} \right)^2, \quad n = 0, 1, \dots, A_- - \frac{1}{2}. \quad (17)$$

It hence follows that bound states exist only for $A_- \geq 1/2$. This is the well-known result for the Morse

potential in one dimension [9], [22]. The corresponding bound-state wave function is

$$\psi_n(x) = \phi_n(x) = G_n y^{-A_- + 1/2} e^{-1/2y} J_n^{-A_-}(y).$$

Using orthogonality property (A.3) of Bessel polynomials, we easily find that $\psi_n(x)$ is orthonormal,

$$\begin{aligned} \langle \psi_n | \psi_m \rangle &= \lambda \int_{-\infty}^{+\infty} \phi_n(x) \phi_m(x) dx = \\ &= G_n G_m \int_0^{\infty} y^{-2A_-} e^{-1/y} J_n^{-A_-}(y) J_m^{-A_-}(y) dy = \delta_{nm}. \end{aligned} \quad (18)$$

Therefore, the finite incomplete basis set whose elements are given by Eq. (3) does give a faithful physical representation for a finite number of bound states of the system whose potential function is given by Eq. (1) with $A_+ = 0$.

As a result of applying the TRA in the general case $A_+ \neq 0$, we now obtain $B_n^\mu(4\varepsilon/A_+; -1/A_+)$, which contains all physical properties of the system [12]. Unfortunately, as noted above, we failed to find analytic properties of this polynomial in the mathematical literature. This remains an open problem in orthogonal polynomials along with other similar problems presented in [23]–[25]. We note that the weak spot in our analysis is that recurrence relation (15) gives the polynomials of any degree in explicit, although not closed, form starting with $B_0^\mu(z; \gamma) = 1$. Nevertheless, we derive a very stable and convergent numerical result.

For example, the Hamiltonian representation in ‘‘Bessel basis’’ (3) is an $N \times N$ tridiagonal symmetric matrix, which is obtained from the three-term recurrence relation for $P_n(4\varepsilon/A_+)$ and has the elements

$$H_{n,m} = \frac{\lambda^2}{8} A_+ (a_n \delta_{n,m} + b_{n-1} \delta_{n,m+1} + b_n \delta_{n,m-1}), \quad n, m = 0, 1, \dots, N-1, \quad (19)$$

where a_n and b_n are obtained from (13) and (14). Diagonalizing this matrix gives the energy spectrum of the lowest bound states.

We list the bound-state energies for several values of A_- and fixed $A_+ = 2$ in Table 1, and we fix $A_- = 6$ and vary A_+ in Table 2. The second column in Table 2 (for $A_+ = 0$) is given to verify the accuracy of our calculations; in it, we reproduced the well-known energy spectrum (17) of the Morse potential.

Table 1

n	$A_- = 8$	$A_- = 6$	$A_- = 4$
0	-28.053627	-15.025220	-5.960092
1	-21.029931	-9.975990	-2.808535
2	-14.992219	-5.880414	-0.106373
3	-9.927105	-2.662228	
4	-5.801982	0.418853	
5	-2.518657		
6	0.948521		

The lowest bound-state energies (in atomic units) corresponding to $A_+ = 2$ for several values of A_- with $\lambda = 1$.

Table 2

n	$A_+ = 0$	$A_+ = 4$	$A_+ = 8$	$A_+ = 12$
0	-15.125000	-14.925872	-14.728422	-14.532562
1	-10.125000	-9.828860	-9.539719	-9.256701
2	-6.125000	-5.645103	-5.195514	-4.765950
3	-3.125000	-2.229669	-1.374691	-0.509143
4	-1.125000	2.004504	5.213347	8.439356

The lowest bound-state energies (in atomic units) corresponding to $A_- = 6$ for several values of A_+ with $\lambda = 1$. The second column with $A_+ = 0$ reproduces the well-known energy spectrum of the Morse potential.

But we repeat that our obtained solution is at best quasi-exact and not exact, i.e., we obtained only a finite part of the energy spectrum and not the whole infinite spectrum (except, of course, in the case $A_+ = 0$, where the spectrum is finite). Moreover, because the size of Hamiltonian matrix (19) is bounded (because $(n, m) \leq N - 1$), we expect that the accuracy of our results is substantially reduced at higher energy levels.

In Appendix B, we independently calculate the energy spectrum by diagonalizing the Hamiltonian matrix in a complete square-integrable basis. For the numerical analysis in this case, we choose a relatively large subset of this basis (i.e., a large matrix size) to produce numbers that are more accurate. We again calculate using the physical parameters in Tables 1 and 2 and present the results in Tables 3 and 4. Comparing these results confirms our supposition that the accuracy in Tables 1 and 2 is substantially reduced at higher energy levels. This again emphasizes that it is important and urgent to obtain the analytic properties of the orthogonal polynomial $B_n^\mu(z; \gamma)$ to be able to obtain an accurate quasi-exact solution of the problem.

Table 3

n	$A_- = 8$	$A_- = 6$	$A_- = 4$
0	-28.053627	-15.025220	-5.960092
1	-21.029931	-9.975990	-2.809728
2	-14.992219	-5.880416	-0.410359
3	-9.927105	-2.667212	1.581097
4	-5.801990	-0.146643	3.496007
5	-2.530695	2.014391	5.470629
6	0.093216	4.103609	7.493054
7	2.391258	6.224812	9.682386

A reproduction of Table 1 using the procedure outlined in Appendix B with the Hamiltonian matrix size 100×100 .

Table 4

n	$A_+ = 0$	$A_+ = 4$	$A_+ = 8$	$A_+ = 12$
0	-15.125000	-14.925872	-14.728422	-14.532562
1	-10.125000	-9.828860	-9.539720	-9.256705
2	-6.125000	-5.645149	-5.196474	-4.770689
3	-3.125000	-2.262598	-1.542214	-0.896463
4	-1.125000	0.549743	1.669961	2.607619
5	-0.125000	3.095928	4.694312	5.962793

A reproduction of Table 2 using the procedure outlined in Appendix B with the Hamiltonian matrix size 100×100 .

Finally, we can use expression (16) to calculate the bound-state wave functions. In Fig. 2, we plot the nonnormalized wave functions corresponding to the lowest part of the spectrum $\{\varepsilon_m\}$ in the first column for $A_- = 8$ in Table 3. For the calculations, we use

$$\psi_m(x) = e^{(-A_- + 1/2)\lambda x} \exp\left(-\frac{1}{2}e^{-\lambda x}\right) \sum_n G_n B_n^{-A_-} \left(\frac{4\varepsilon_m}{A_+}; -\frac{4}{A_+}\right) J_n^{-A_-}(e^{\lambda x}). \quad (20)$$

To see the features of the wave function, we superimposed the potential (not to scale) on the same plots and indicated the corresponding energy level with a horizontal dotted line.

Interesting confinement features of the potential can be seen in the plots of the wave functions. First, the wave function does not decrease abruptly at the walls of the potential well but exhibits some penetration with a rapidly decaying tail, which is shorter on the left than on the right because the confinement $e^{-2\lambda x}$ on the left is stronger than $e^{\lambda x}$ on the right. Second, the wave function for low energies apparently bunches at the left side of the well, where it is deeper. Third, the particle at higher energies does not “feel” the topography at the bottom of the well and oscillates, but at these higher energies, the particle still feels the weaker right wall and tends to cluster there.

Appendix A: Bessel polynomials on the real line

Bessel polynomials on the real line are defined in terms of the hypergeometric or confluent hypergeometric functions as (see Sec. 9.13 in [18])

$$J_n^\mu(x) = {}_2F_0\left(-n, n + \underline{2}\mu + 1 \mid -x\right) = (n + 2\mu + 1)_n x^n {}_1F_1\left(\begin{matrix} -n \\ -2(n + \mu) \end{matrix} \mid \frac{1}{x}\right), \quad (A.1)$$

where $n = 0, 1, \dots, N$ and N is a nonnegative integer. The real parameter μ is negative such that $\mu < -N - 1/2$. The Pochhammer symbol $(a)_n$ (also called a shifted factorial) is defined as $a(a+1)(a+2)\cdots(a+n-1) = \Gamma(n+a)/\Gamma(a)$. The Bessel polynomial can also be written in terms of the associated Laguerre polynomial with a discrete index as $J_n^\mu(x) = n!(-x)^n L_n^{-(2n+2\mu+1)}(1/x)$. The three-term recurrence relation is

$$\begin{aligned} 2xJ_n^\mu(x) = & -\frac{\mu}{(n+\mu)(n+\mu+1)}J_n^\mu(x) - \frac{n}{(n+\mu)(2n+2\mu+1)}J_{n-1}^\mu(x) + \\ & + \frac{n+2\mu+1}{(n+\mu+1)(2n+2\mu+1)}J_{n+1}^\mu(x). \end{aligned} \quad (A.2)$$

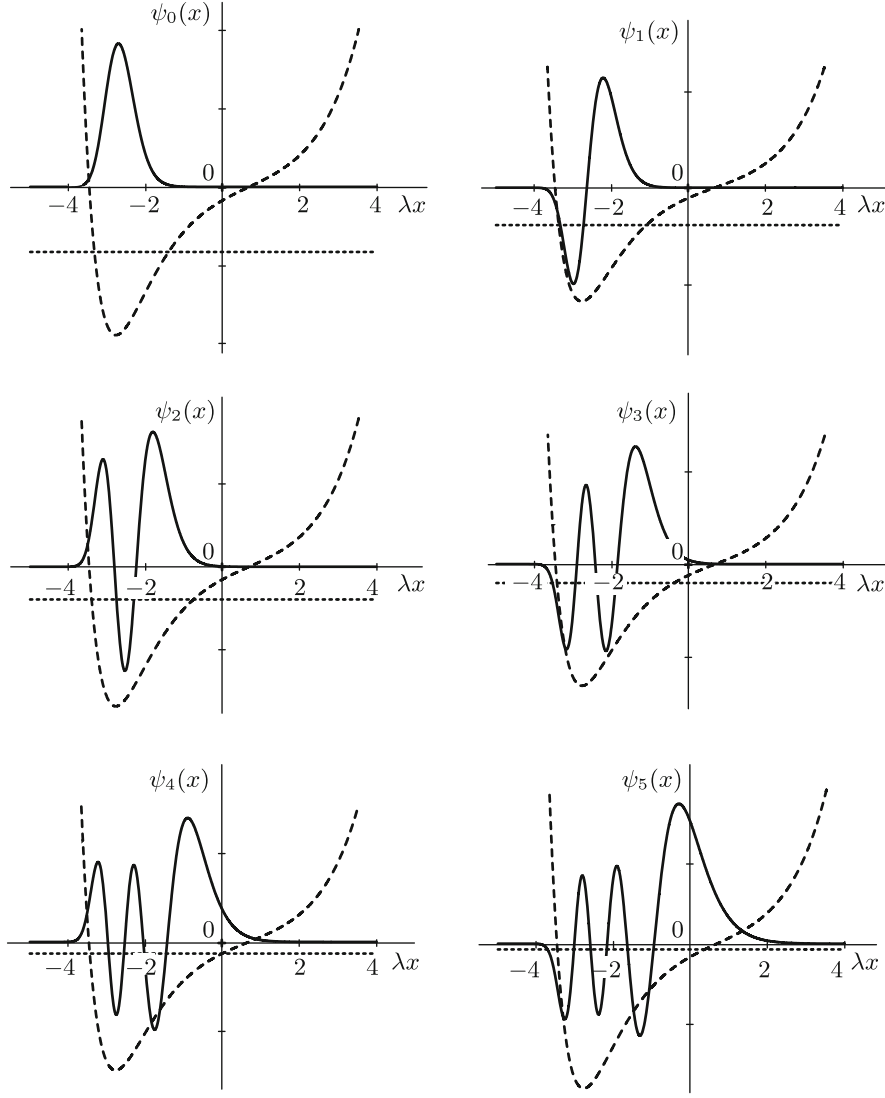


Fig. 2. Nonnormalized wave functions $\psi_n(x)$, $n = 0, 1, \dots, 5$, corresponding to the energies shown in the first column of Table 3 where $A_+ = 2$ and $A_- = 8$: the potential function (dashed curve) is superimposed on the same plot (not to scale), and the corresponding energy level is indicated by the horizontal dotted line.

We note that the constraints on μ and on the polynomial degree make this recursion definite (i.e., the signs of the two recursion coefficients multiplying $J_{n\pm 1}^\mu(x)$ are the same). Otherwise, these polynomials would be orthogonal not on the real line but on the unit circle in the complex plane. The orthogonality relation is

$$\int_0^\infty x^{2\mu} e^{-1/x} J_n^\mu(x) J_m^\mu(x) dx = -\frac{n! \Gamma(-n - 2\mu)}{2n + 2\mu + 1} \delta_{nm}. \quad (\text{A.3})$$

The differential equation is

$$\left\{ x^2 \frac{d^2}{dx^2} + [1 + 2x(\mu + 1)] \frac{d}{dx} - n(n + 2\mu + 1) \right\} J_n^\mu(x) = 0. \quad (\text{A.4})$$

The forward shift and the backward shift differential relations are

$$\frac{d}{dx} J_n^\mu(x) = n(n+2\mu+1)J_{n-1}^{\mu+1}(x), \quad (\text{A.5})$$

$$x^2 \frac{d}{dx} J_n^\mu(x) = -(2\mu x + 1)J_n^\mu(x) + J_{n+1}^{\mu-1}(x). \quad (\text{A.6})$$

We can write $J_{n+1}^{\mu-1}(x)$ in terms of $J_n^\mu(x)$ and $J_{n\pm 1}^\mu(x)$ as

$$\begin{aligned} 2J_{n+1}^{\mu-1}(x) &= \frac{(n+1)(n+2\mu)}{(n+\mu)(n+\mu+1)} J_n^\mu(x) + \frac{n(n+1)}{(n+\mu)(2n+2\mu+1)} J_{n-1}^\mu(x) + \\ &+ \frac{(n+2\mu)(n+2\mu+1)}{(n+\mu+1)(2n+2\mu+1)} J_{n+1}^\mu(x). \end{aligned} \quad (\text{A.7})$$

Using this identity and recurrence relation (A.2), we can rewrite the backward shift differential relation as

$$\begin{aligned} 2x^2 \frac{d}{dx} J_n^\mu(x) &= n(n+2\mu+1) \left[-\frac{J_n^\mu(x)}{(n+\mu)(n+\mu+1)} + \frac{J_{n-1}^\mu(x)}{(n+\mu)(2n+2\mu+1)} + \right. \\ &\left. + \frac{J_{n+1}^\mu(x)}{(n+\mu+1)(2n+2\mu+1)} \right]. \end{aligned} \quad (\text{A.8})$$

The generating function is

$$\sum_{n=0}^{\infty} J_n^\mu(x) \frac{t^n}{n!} = \frac{2^{2\mu}}{\sqrt{1-4xt}} (1 + \sqrt{-4xt})^{-2\mu} \exp\left[\frac{2t}{1 + \sqrt{1-4xt}} \right]. \quad (\text{A.9})$$

Appendix B: Alternative evaluation of the energy spectrum

In this appendix, we obtain an independent and more accurate numerical evaluation of the energy spectrum associated with exponential potential well (1) by diagonalizing the Hamiltonian matrix in an appropriate discrete square-integrable basis. We choose basis functions forming the so-called Laguerre basis,

$$\phi_n(x) = A_n y^\alpha e^{-y/2} L_n^\nu(y), \quad (\text{B.1})$$

where $L_n^\nu(y)$ is the Laguerre polynomial and the normalization constant is $A_n = \sqrt{n!/\Gamma(n+\nu+1)}$. We transform the coordinate as $y(x) = e^{-\lambda x}$, the inverse to transformation (3) in the ‘‘Bessel basis.’’ The real parameters α and ν are chosen below; here, we note that $\nu > -1$. In the atomic units $\hbar = M = 1$, the Hamiltonian operator is

$$H = -\frac{1}{2} \frac{d^2}{dx^2} + V(x) = -\frac{\lambda^2}{2} \left[y^2 \frac{d^2}{dy^2} + y \frac{d}{dy} - W(y) \right], \quad (\text{B.2})$$

where

$$W(y) = \frac{2V(x)}{\lambda^2} = \frac{1}{4} y^2 - A_- y + A_+ y^{-1}.$$

Using the differential equation for the Laguerre polynomials

$$\left[y \frac{d^2}{dy^2} + (\nu+1-y) \frac{d}{dy} + n \right] L_n^\nu(y) = 0,$$

we obtain the action of the operator H on the basis elements

$$-\frac{2}{\lambda^2}H|\phi_n\rangle = A_n y^\alpha e^{-y/2} \left[(2\alpha - \nu)y \frac{d}{dy} + \frac{y^2}{4} - \left(n + \alpha + \frac{1}{2} \right) y + \alpha^2 - W(y) \right] |L_n^\nu\rangle. \quad (\text{B.3})$$

Applying the differential formula for the Laguerre polynomials

$$y \frac{dL_n^\nu}{dy} = nL_n^\nu - (n + \nu)L_{n-1}^\nu \quad (\text{B.4})$$

and the explicit expression for $W(y)$, we obtain

$$-\frac{2}{\lambda^2}H|\phi_n\rangle = A_n y^\alpha e^{-y/2} \left\{ (\nu - 2\alpha)(n + \nu) |L_{n-1}^\nu\rangle + \left[\alpha^2 + n(2\alpha - \nu) - \left(n + \alpha + \frac{1}{2} - A_- \right) y - \frac{A_+}{y} \right] |L_n^\nu\rangle \right\}.$$

Let the integral measure be defined as $\lambda \int_{-\infty}^{+\infty} (\cdot) dx = \int_0^\infty (\cdot) y^{-1} dy$. Then the matrix elements of the Hamiltonian in Laguerre basis (B.1) have the form

$$-\frac{2}{\lambda^2} \langle \phi_m | H | \phi_n \rangle = A_m A_n (\nu - 2\alpha)(n + \nu) \langle L_m^\nu | y^{2\alpha-1} e^{-y} | L_{n-1}^\nu \rangle + A_m A_n \langle L_m^\nu | y^{2\alpha-1} e^{-y} \left[\alpha^2 + n(2\alpha - \nu) - \left(n + \alpha + \frac{1}{2} - A_- \right) y - \frac{A_+}{y} \right] | L_n^\nu \rangle. \quad (\text{B.5})$$

If we introduce

$$\langle m | f(y) | n \rangle = A_m A_n \langle L_m^\nu | y^\nu e^{-y} f(y) | L_n^\nu \rangle = A_m A_n \int_0^\infty y^\nu e^{-y} f(y) L_m^\nu(y) L_n^\nu(y) dy.$$

then we obtain

$$-\frac{2}{\lambda^2} \langle \phi_m | H | \phi_n \rangle = (\nu - 2\alpha) \sqrt{n(n + \nu)} \langle m | y^{2\alpha-\nu-1} | n-1 \rangle + \langle m | y^{2\alpha-\nu-1} \left[\alpha^2 + n(2\alpha - \nu) - \left(n + \alpha + \frac{1}{2} - A_- \right) y - \frac{A_+}{y} \right] | n \rangle. \quad (\text{B.6})$$

Using the orthogonality of the Laguerre polynomials,

$$A_m A_n \int_0^\infty y^\nu e^{-y} L_m^\nu(y) L_n^\nu(y) dx = \delta_{m,n},$$

and choosing $2\alpha = \nu + 1$, we obtain

$$-\frac{2}{\lambda^2} \langle \phi_m | H | \phi_n \rangle = -\sqrt{n(n + \nu)} \delta_{m,n-1} + \left[n + \frac{1}{4}(\nu + 1)^2 \right] \delta_{m,n} - \left(n + \frac{\nu}{2} + 1 - A_- \right) \langle m | y | n \rangle - A_+ \langle m | y^{-1} | n \rangle. \quad (\text{B.7})$$

Applying the three-term recurrence relation for Laguerre polynomials

$$yL_n^\nu = (2n + \nu + 1)L_n^\nu - (n + \nu)L_{n-1}^\nu - (n + 1)L_{n+1}^\nu$$

and their orthogonality relation, we obtain the tridiagonal symmetric matrix representation for $\langle m|y|n\rangle$:

$$\langle m|y|n\rangle = (2n + \nu + 1)\delta_{m,n} - \sqrt{n(n + \nu)}\delta_{m,n-1} - \sqrt{(n + 1)(n + \nu + 1)}\delta_{m,n+1} := T_{m,n}. \quad (\text{B.8})$$

On the other hand, we can use any approximation method to evaluate the integral $\langle m|y^{-1}|n\rangle$. Applying the Gauss method [26]–[29] for Laguerre polynomials, we obtain

$$\langle m|y^{-1}|n\rangle \cong \sum_{k=0}^{K-1} \frac{1}{\xi_k} \Lambda_{m,k} \Lambda_{n,k}, \quad (\text{B.9})$$

where $\{\xi_k\}_{k=0}^{K-1}$ is the set of eigenvalues of the $K \times K$ tridiagonal symmetric matrix T given by (B.8) and $\{\Lambda_{m,k}\}_{m=0}^{K-1}$ are the normalized eigenvectors corresponding to these eigenvalues.

To obtain a representation of the Hamiltonian H as a $K \times K$ matrix with elements (B.7), we now only need to assign a value to the basis parameter ν for any given set $\{\lambda, A_{\pm}\}$ of potential parameters. We assume that the physical results are independent of the choice of ν .

We choose a value for ν within a range, called the “stability plateau,” where the obtained results do not significantly deviate (in the limits of the required accuracy) from the exactly known energy spectrum of the Morse potential for $A_+ = 0$. This plateau widens as the size of the matrix H increases, i.e., the range from which we can choose a “good” value of ν increases as K increases. Ideally, the size of the plateau becomes infinite as $K \rightarrow \infty$. In other words, the results are independent of ν for $\nu > -1$. Finally, we choose $\nu = 0$.

We also note that with $2\alpha = \nu + 1$, the basis becomes orthonormalized (i.e., $\langle \phi_m | \phi_n \rangle = \delta_{m,n}$). We could also obtain the energy spectrum with other relations between the basis parameters α and ν . For example, we could choose $2\alpha = \nu$ or $2\alpha = \nu + 2$ with the corresponding matrices $\langle \phi_m | \phi_n \rangle = \langle m|y^{-1}|n\rangle$ and $\langle \phi_m | \phi_n \rangle = \langle m|y|n\rangle$. We choose $2\alpha = \nu + 1$ because for the same basis size, the coincidence with the exact energy spectrum of the Morse potential is closer in this case than with the other two variants.

We again calculated with the physical parameters in Tables 1 and 2, using the procedure described above with $2\alpha = \nu + 1$ and $K = 100$; we present the results in Tables 3 and 4.

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