

## Exact wave-function normalization constants for the $B_0 \tanh z - U_0 \cosh^{-2} z$ and Pöschl-Teller potentials

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We obtain, in exact closed form, the wave-function normalization constants for the Schrödinger equation with potential  $V = B_0 \tanh z - U_0 \cosh^{-2} z$ . These constants are derived in terms of a variety of formulations and solutions of the equation. We give discussions of both mathematical aspects and physical motivations of the problem. The main results are gathered in two appendixes. Wave-function normalization constants for the related Pöschl-Teller potential are given in a third appendix.

### I. INTRODUCTION

In 1932 Rosen and Morse<sup>1</sup> (RM) found the exact energy eigenvalues and unnormalized eigenfunctions of the Schrödinger equation

$$\left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x)\right) \psi = E \psi \tag{1.1}$$

for the potential

$$V(x) = B_0 \tanh \alpha x - U_0 \cosh^{-2} \alpha x. \tag{1.2}$$

This potential has a minimum at

$$x_0 = -\alpha^{-1} \tanh^{-1}(B_0/2U_0) \tag{1.3}$$

with value

$$V(x_0) = -(U_0 + B_0^2/4U_0) \tag{1.4}$$

and is shown schematically in Fig. 1. Rosen and Morse were also interested in matching two of these potentials end to end (one reversed) for use as a model of one-dimensional double-well potentials. Such potentials were appropriate to certain polyatomic molecules along given axes. (Of course, during the first decade of quantum mechanics, as well as later, many studies were done on exactly solvable and approximately solvable potential problems. See, for example, Refs. 1-10.)

When the potential of Eq. (1.2) is specialized to the symmetric case ( $B_0 = 0$ )

$$V = -U_0 \cosh^{-2} \alpha x, \tag{1.5}$$

there are additional reasons for interest in it. Equation (1.5) is a potential which occurs in the study of solitons.<sup>11</sup> Also (see Sec. IIIA below), the three-dimensional radial form of Eq. (1.5) ( $x \rightarrow r$ ) is exactly solvable for the  $L = 0$  case, and thus is also a useful model potential.

Although the potentials of Eqs. (1.2) and (1.5) are important enough to be found as standard quantum-mechanics examples in, for example, Refs. 12 and 13, respectively, in none of the dis-

cussions we have mentioned have the wave-function normalization constants been given in closed form.<sup>14</sup> A reason is that in terms of the standard solutions, the normalization constants turn out to be double sums of products of 11 gamma functions with changing signs.

It is the purpose of this paper to give these normalization constants in exact closed form. In addition to the desirability, in itself, of having these constants for the number states, with these constants one could in principle go on to investigate the coherent states for this system. We will return to this point in Sec. V.

In Sec. II we begin by deriving the normalization constants for the symmetric case (1.5), using the discussion of Landau and Lifshitz<sup>13</sup> (LL). The advantage of their notation is that the problem splits up into two calculations, for the even and odd states. This is especially useful when one continues to the three-dimensional case, since there only the odd states survive. We will find

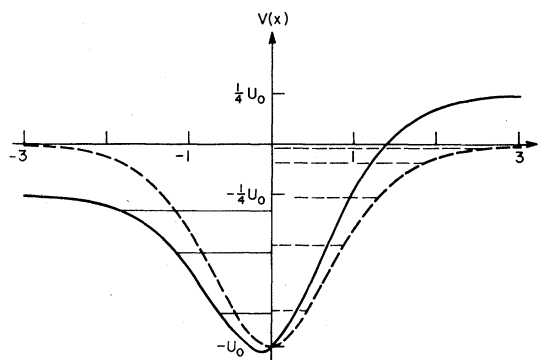


FIG. 1. Solid line shows the complete potential of Eq. (1.2) plotted with  $x$  in units of  $1/\alpha$  and for  $B_0 = \frac{1}{4} U_0$ . The dashed line shows the  $B_0 = 0$  symmetric potential of Eq. (1.5). For  $U_0 = \frac{29}{8} \alpha^2 \hbar^2/m$ , the five horizontal dashed lines are the bound-state energy levels for the symmetric potential and the three horizontal solid lines are the bound-state energy levels for the complete potential.

that the normalization constants can be obtained by transforming the standard hypergeometric function solutions into Jacobi polynomials and thus using certain changes of variables and known integrals.

In Sec. III we proceed to the entire potential of Eq. (1.2) in terms of the original Rosen and Morse discussion.<sup>1</sup> The calculation of the normalization constants is similar to but slightly more complicated than that of Sec. II. In the limit as  $B_0 \rightarrow 0$  these normalizations are consistent with those obtained in Sec. II. We also give the transformation to the Morse and Feshbach<sup>12</sup> (MF) notation.

Section IV contains a mathematical discussion. We first describe the modification which allows one to write the above normalization constants for wave functions in terms of Jacobi polynomials. Next, we observe that, for the symmetric potential of Eq. (1.5), the normalized wave functions can also be given first in terms of Gegenbauer polynomials and finally in terms of associated Legendre functions. In particular, we observe that the normalized wave functions for the complete potential (in terms of Jacobi polynomials) and for the symmetric potential (in terms of associated Legendre functions) are particularly simple. As Simmons has observed, the basis for this is that the original Schrödinger equation can be transformed into Riemann's equation, which then directly has the mentioned simple solutions.

We then point out the connection of our explicit RM normalized wave functions for the complete potential (1.2) to the implicit normalized wave functions for that potential which can be generated by the factorization method as described by Infeld and Hull.<sup>15</sup>

Finally, in Sec. V, we discuss the possible application of our results to finding the coherent states of this system, either by analytic or group-theory means. These coherent states could possibly be of use for the forced-oscillator problem.

In Appendixes A and B we gather some special-case solutions and all our general results, respectively.

In Appendix C, we give the normalized wave-function results for the related Pöschl-Teller potential

$$V(x) = \frac{\hbar^2 \alpha^2}{2m} \left( \frac{\kappa(\kappa-1)}{\sin^2 \alpha x} + \frac{\lambda(\lambda-1)}{\cos^2 \alpha x} \right), \quad \kappa, \lambda > 1. \quad (1.6)$$

## II. SYMMETRIC POTENTIAL, $B_0 = 0$

### A. One-dimensional case

For the symmetric case of Eq. (1.5) we find it most illuminating to use the notation of Landau and Lifshitz.<sup>13</sup> One starts from the Schrödinger equation

$$\left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} - \frac{U_0}{\cosh^2 \alpha x} \right) \psi = E \psi, \quad (2.1)$$

and rewrites the wave function in the form

$$\psi(x) = \frac{N\omega(x)}{\cosh^s \alpha x}, \quad s = \frac{1}{2} \left[ -1 + \left( 1 + \frac{8mU_0}{\alpha^2 \hbar^2} \right)^{1/2} \right]. \quad (2.2)$$

By next defining

$$q = \sinh^2 \alpha x, \quad \epsilon = (-2mE)^{1/2} \geq 0, \quad (2.3)$$

one obtains from the above an equation for  $\omega$ . From Eq. (15.5.1) of Abramowitz and Stegun<sup>16</sup> (AS), the solution is a hypergeometric function. Specifically, in our case one has energy levels  $E_n$  ( $n=0, 1, 2, \dots$ ) determined by

$$n = s - \epsilon(n), \quad s^2 - \epsilon^2 = n(2s - n), \quad (2.4)$$

or

$$E_n = -\frac{\hbar^2 \alpha^2}{8m} \left[ -(1+2n) + \left( 1 + \frac{8mU_0}{\alpha^2 \hbar^2} \right)^{1/2} \right]^2. \quad (2.5)$$

The solutions  $\omega_E$  and  $\omega_0$  for even and odd  $n$  are [see Eqs. (15.5.3) and (15.5.4) of AS<sup>16</sup>]

$$\omega_E = F\left(-\frac{1}{2}n, \frac{1}{2}n - s; \frac{1}{2}; -\sinh^2 \alpha x\right), \quad n = 0, 2, 4, \dots, \quad (2.6)$$

$$\omega_0 = \sinh \alpha x F\left(-\frac{1}{2}(n-1), \frac{1}{2}(n-1) - s + 1; \frac{3}{2}; -\sinh^2 \alpha x\right), \quad n = 1, 3, 5, \dots \quad (2.7)$$

Note that Eqs. (2.2), (2.4), and (2.5) imply that there is always at least one bound state ( $n=0$ ) for any  $U_0 > 0$ , no matter how small.

We now proceed to find the normalization constants  $N(n)$ . When the first label in a hypergeometric function is a negative integer, then the hypergeometric function can be given by a finite power series. By using Eq. (15.4.1) of AS<sup>16</sup> one can write [see Eq. (15.5.3) of AS<sup>16</sup>] the even solutions as

$$\psi_E(n=0, 2, 4, \dots) = \frac{N_E(n)}{(\cosh \alpha x)^s} \omega_E(n), \quad (2.8)$$

$$\omega_E(n) = \sum_{j=0}^{n/2} A(j, n, s) (\sinh \alpha x)^{2j}, \quad (2.9a)$$

$$A(j, n, s) \equiv \frac{\Gamma(\frac{1}{2}n+1)}{\Gamma(\frac{1}{2}n-j+1)} \frac{\Gamma(s-\frac{1}{2}n+1)}{\Gamma(s-\frac{1}{2}n-j+1)} \times \frac{\Gamma(\frac{1}{2})}{\Gamma(\frac{1}{2}+j)} \frac{(-1)^j}{\Gamma(j+1)}, \quad (2.9b)$$

and the odd solutions as [see Eq. (15.5.4) of AS<sup>16</sup>]

$$\psi_O(n=1, 3, 5, \dots) = \frac{N_O(n)}{(\cosh \alpha x)^s} \omega_O(n), \quad (2.10)$$

$$\omega_O(n) = \sinh \alpha x \sum_{j=0}^{\frac{1}{2}(n-1)} C(j, n, s) (\sinh \alpha x)^{2j}, \quad (2.11a)$$

$$C(j, n, s) \equiv \frac{\Gamma(\frac{1}{2}(n-1)+1)}{\Gamma(\frac{1}{2}(n-1)-j+1)} \frac{\Gamma(s-\frac{1}{2}(n-1))}{\Gamma(s-\frac{1}{2}(n-1)-j)} \times \frac{\Gamma(\frac{3}{2})}{\Gamma(\frac{3}{2}+j)} \frac{(-1)^j}{\Gamma(j+1)}. \quad (2.11b)$$

The above mean that the even and odd normalization constants, obtained from integrating  $\omega^2(\cosh\alpha x)^{-2s}$ , are given by

$$N_B^{-2} = \frac{1}{\alpha} \sum_{\substack{j=0 \\ k=0}}^{n/2} A(j, n, s) A(k, n, s) \\ \times B(j+k+\frac{1}{2}, s-j-k), \quad (2.12)$$

$$N_O^{-2} = \frac{1}{\alpha} \sum_{\substack{j=0 \\ k=0}}^{(n-1)/2} C(j, n, s) C(k, n, s) \\ \times B(j+k+\frac{3}{2}, s-j-k-1), \quad (2.13)$$

where  $B(a, b)$  is the beta function  $B(a, b) = \Gamma(a)\Gamma(b)/\Gamma(a+b)$ . The beta functions in (2.12) and (2.13) arise from integrals of the form

$$\int_0^\infty \frac{\sinh^\mu x}{\cosh^\nu x} dx = \frac{1}{2} B\left(\frac{\mu+1}{2}, \frac{\nu-\mu}{2}\right), \\ [\operatorname{Re}\nu > -1, \operatorname{Re}(\mu-\nu) < 0] \quad (2.14)$$

given in (3.512.2) of Gradshteyn and Ryzhik<sup>17,18</sup> (GR).

The normalization constants (2.12) and (2.13) are, in addition to other numerical factors, double sums of products of 11 gamma functions of  $j$  and  $k$ , with changing signs. However, they can be evaluated as we show below. First we state the results, which are also listed in Appendix B.

$$\alpha N_B^{-2} = \frac{1}{2} (n+1) B\left(\frac{1}{2}, s-\frac{1}{2}n\right) B\left(\frac{1}{2}, \frac{1}{2}n+1\right) \\ \times \left(\frac{s-\frac{1}{2}n}{s-n}\right), \quad (2.15)$$

$$\alpha N_O^{-2} = \frac{1}{2} B\left(\frac{3}{2}, s-\frac{1}{2}(n+1)\right) B\left(\frac{1}{2}, \frac{1}{2}(n+1)\right) \\ \times \left(\frac{s-\frac{1}{2}(n+1)}{s-n}\right). \quad (2.16)$$

We have checked these normalization formulas explicitly for the special cases up to  $n=8$  by comparing with the double-sum formulas (2.12) and (2.13). (The complete explicit wave functions are given in Appendix A up to  $n=8$ .) Further note that if one has a zero-energy solution given by  $s=n$ , the denominators of the last factors in Eqs. (2.15) and (2.16) show that this solution is not normalizable, but rather is part of the continuum.

Now we shall prove the even case, (2.15). Change variables in the normalization integral from  $x$  to  $z = \alpha x$  and then change the limits of integration from  $(-\infty, \infty)$  to  $(0, \infty)$ . Next one uses one of the formulas relating a hypergeometric function with a negative integer first argument to a Jacobi polynomial. Specifically, using the identifications

$$\frac{X+1}{X-1} = -\sinh^2 z, \quad y = \tanh^2 z, \quad (2.17a)$$

$$N = \frac{1}{2}n, \quad \alpha = s-n, \quad \beta = -\frac{1}{2}, \quad (2.17b)$$

in Eq. (25.5.45) of AS<sup>16</sup> and then changing variables from  $z$  to  $y$  yields

$$F\left(-\frac{1}{2}n, \frac{1}{2}n-s; \frac{1}{2}; -\sinh^2 z\right) \\ = \frac{\Gamma(\frac{1}{2}n+1)\Gamma(\frac{1}{2})}{\Gamma(\frac{1}{2}n+\frac{1}{2})} (y-1)^{-n/2} P_{n/2}^{(s-n, -1/2)}(2y-1). \quad (2.18)$$

Now a further change of variables,

$$t = 2y-1, \quad (2.19)$$

yields

$$\alpha N_B^{-2}(n) \\ = \int_{-1}^1 dt (1-t)^{s-n-1} (1+t)^{-1/2} [P_{n/2}^{(s-n, -1/2)}(t)]^2 \\ \times \left(\frac{\Gamma(\frac{1}{2})\Gamma(\frac{1}{2}n+1)}{\Gamma(\frac{1}{2}n+\frac{1}{2})}\right)^2 2^{-s+n+1/2}. \quad (2.20)$$

One finally uses Eq. (7.391.5) of GR<sup>17</sup>

$$\int_{-1}^1 (1-x)^{\alpha-1} (1+x)^\beta [P_n^{(\alpha, \beta)}(x)]^2 dx \\ = \frac{2^{\alpha+\beta} \Gamma(\alpha+n+1)\Gamma(\beta+n+1)}{(n!) \alpha \Gamma(\alpha+\beta+n+1)} \quad (2.21)$$

to obtain the final answer. Note that the  $\alpha$  in the denominator on the right of (2.21) is where the factor  $1/(s-n)$  in (2.15) comes from, this factor yielding the result that a zero-energy eigenvector is not normalizable.

With one slight modification, the odd normalization constants  $N_O$  of Eq. (2.16) are calculated the same way. The difference is that this time the identifications (2.17b) are modified to

$$N = \frac{1}{2}(n-1), \quad \alpha = s-n, \quad \beta = \frac{1}{2}, \quad (2.22)$$

so that

$$F\left(-\frac{1}{2}(n-1), \frac{1}{2}(n-1)-s+1; \frac{3}{2}; -\sinh^2 z\right) \\ = \frac{\Gamma(\frac{1}{2}(n+1))\Gamma(\frac{3}{2})}{\Gamma(\frac{1}{2}n+1)} (y-1)^{-(n-1)/2} \\ \times P_{(n-1)/2}^{(s-n, 1/2)}(2y-1). \quad (2.23)$$

The rest of the calculation proceeds similarly to that for  $N_B$ .

### B. Three-dimensional case

When one considers the three-dimensional problem  $x \rightarrow r$  then one can factor out the angular and radial wave functions in the usual manner,<sup>19</sup> obtaining from

$$\psi_{\rho l m} = N_R(\rho, l) R_{\rho l} Y_{l m}, \quad R_{\rho l} \equiv \chi_{\rho l} / r, \quad (2.24)$$

the equation for  $\chi$  of

$$\left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial r^2} - \frac{U_0}{\cosh^2 \alpha r} + \frac{l(l+1)\hbar^2}{2mr^2} \right) \chi_{\rho l} = E_{\rho l} \chi_{\rho l}. \quad (2.25)$$

For the S-wave ( $l=0$ ) case, this equation for  $\chi_{\rho 0}$  is exactly the same as the one-dimensional equation (2.1). The only complication is that, since the complete wave function must have continuous derivatives at the origin, we must rule out the even solutions,  $n=0, 2, \dots$ , which go to infinity at the origin, and keep only the odd solutions,  $n=1, 3, \dots$ , of the form (2.10), which go to zero at the origin.<sup>20</sup> A consequence is that there is not always a bound state in the three-dimensional problem. One needs to have

$$mU_0/\alpha^2\hbar^2 \geq 1 \quad (2.26)$$

for there to exist a bound state. The normalization constants  $N_{R}(\rho, 0)$  differ from the odd normalization constants (2.16) by a factor of  $\sqrt{2}$  because the radial integral in three dimensions only goes from zero to infinity. To summarize:

$$E_{\rho 0} = \frac{-\hbar^2\alpha^2}{8m} \left[ -[1+2(2\rho+1)] + \left( 1 + \frac{8mU_0}{\alpha^2\hbar^2} \right)^{1/2} \right], \quad (2.27)$$

$$N_{R}(\rho, 0) = \sqrt{2} N_{O}(2\rho+1), \quad \rho=0, 1, 2, \dots$$

Since for physical problems the rotational excitations are usually small compared to the radial excitations, one can use perturbation theory to discuss the modifications necessary for  $l \neq 0$ .<sup>21</sup>

### III. COMPLETE POTENTIAL

#### A. Normalization constants

For the complete potential of (1.2), we found it clarifying to use the original formulation of Rosen and Morse.<sup>1</sup> In their discussion they eventually obtain a hypergeometric expansion in terms of the variable

$$u = \frac{e^z}{e^z + e^{-z}} = \frac{1}{2} (1 + \tanh z), \quad z \equiv \alpha x, \quad (3.1)$$

instead of the LL expansion in  $\sinh \alpha x$  of Sec. II. The discussion of the derivation of the energy levels and wave functions is similar to that of Sec. II, and need not be repeated. The reader can simply verify that the eigenvalues and solutions to the Schrödinger equation with the complete potential (1.2) is

$$E_n = -\frac{\hbar^2\alpha^2}{8m} D_n^2 - \frac{2mB_0^2}{\alpha^2\hbar^2 D_n^2}, \quad (3.2)$$

$$D_n = -(1+2n) + \left( 1 + \frac{8mU_0}{\alpha^2\hbar^2} \right)^{1/2} = 2(s-n), \quad (3.3)$$

$$0, 1, 2, \dots = n \leq s - \left( \frac{mB_0}{\alpha^2\hbar^2} \right)^{1/2}, \quad (3.4)$$

$$\psi_n = N_{RM}(n) e^{a\alpha z} (\cosh^{-s+n} z) \times F(-n, 2s-n+1; s-n+a+1; u), \quad (3.5)$$

where the quantities involved in Eqs. (3.2)–(3.5) are defined so as to closely correspond to the notation of Sec. II when  $B_0=0$ :

$$s = \frac{1}{2} [-1 + (1 + 8mU_0/\alpha^2\hbar^2)^{1/2}], \quad (3.6)$$

$$a = mU_0/[\alpha^2\hbar^2(s-n)]. \quad (3.7)$$

Note that Eq. (3.4) implies that if the potential becomes too skew then it is not possible to have any bound states.

This time, using the fact that

$$F(-n, 2s-n+1; s-n+a+1; u) = \sum_{j=0}^n \frac{\Gamma(n+1)}{\Gamma(n-j+1)} \frac{\Gamma(s-n+a+1)}{\Gamma(2s-n+1)} \times \frac{\Gamma(2s-n+j+1)}{\Gamma(s-n+a+j+1)} \frac{(-u)^j}{\Gamma(j+1)} \quad (3.8)$$

plus the integral (3.512.1) of GR,<sup>17</sup> one finds that

$$\alpha N_{RM}^{-2} = \int_{-\infty}^{\infty} \frac{dz F^2 e^{2az}}{\cosh^{2s-2n} z} \quad (3.9)$$

yields

$$\alpha N_{RM}^{-2} = \frac{1}{2} \sum_{j=0}^n \sum_{k=0}^n H(s, n, a, j) H(s, n, a, k) \times B(s-n+a+j+k, s-n-a), \quad (3.10)$$

$H(s, n, a, j)$

$$= \frac{2^{s-n} \Gamma(n+1) \Gamma(s-n+a+1) \Gamma(2s-n+j+1)}{\Gamma(n-j+1) \Gamma(s-n+a+j+1) \Gamma(2s-n+1)} \times \frac{(-1)^j}{\Gamma(j+1)}. \quad (3.11)$$

To obtain the closed-form normalization constants one considers, as before, the integral (3.9), but this time with the hypergeometric functions transformed to Jacobi polynomials by formula (22.5.42) of AS. One obtains

$$F(-n, 2s-n+1; s-n+a+1; u) = \frac{\Gamma(n+1) \Gamma(s-n+a+1)}{\Gamma(s+a+1)} P_n^{(s-n+a, s-n-a)}(1-2u). \quad (3.12)$$

By inserting (3.12) and (3.5) into (3.9) and then changing variables first to  $u$ , then to  $t=1-2u = (-\tanh z)$ , one ends up with

$$\alpha N_{\text{RM}}^{-2} = \left( \frac{\Gamma(n+1)\Gamma(s-n+a+1)}{\Gamma(s+a+1)} \right)^2 \times \int_{-1}^1 dt (1-t)^{s-n+a-1} (1+t)^{s-n-a-1} \times [P_n^{(s-n+a, s-n-a)}(t)]^2. \quad (3.13)$$

The integral in (3.13) contains an integrand of the form  $(1-t)^{\alpha-1}(1+t)^{\beta-1}[P_n^{(\alpha, \beta)}(t)]^2$ . By multiplying this integrand by 1 in the form

$$1 = \frac{1}{2} [(1+t) + (1-t)], \quad (3.14)$$

(3.13) can be transformed into the two integrals (16.4.11) and (16.4.15) of Ref. 22. When this is done, one is left with the final answer (also see Appendix B)

$$\alpha N_{\text{RM}}^{-2} = 2^{2s-2n} (s-n) \frac{\Gamma(n+1)\Gamma(s-a+1)}{\Gamma(2s-n+1)\Gamma(s+a+1)} \times \frac{\Gamma^2(s-n+a+1)}{(s-n+a)(s-n-a)} \quad (3.15) \\ = \frac{\Gamma(\frac{1}{2}n+\frac{1}{2})\Gamma(s-n+a)}{\Gamma(s-\frac{1}{2}n+\frac{1}{2})} \frac{\Gamma(\frac{1}{2}n+1)\Gamma(s-n-a)}{\Gamma(s-\frac{1}{2}n+1)} \\ \times (s-n) \frac{\Gamma(s-n+a+1)}{\Gamma(s-n-a+1)} \frac{\Gamma(s-a+1)}{\Gamma(s+a+1)}. \quad (3.16)$$

We have checked Eq. (3.16) for the special cases  $n=0, 1, 2$  by calculating these special case results with the double-sum formula (3.10).

#### B. Comparison with the symmetric limit

When one considers the symmetric limit  $B_0=0$ , which means that  $a=0$ , Eq. (3.16) reduces to

$$\alpha N_{\text{RM}}^{-2} \Big|_{a=0} = B(\frac{1}{2}n+\frac{1}{2}, s-n)B(\frac{1}{2}n+1, s-n)(s-n). \quad (3.17)$$

The question arises if this single formula agrees with the separate LL normalization constants (2.15) and (2.16) for the even and odd states. The answer is positive.

Recall that in the LL discussion the wave functions are the hypergeometric functions (2.9) and (2.11) expressed as a power series in  $\sinh z$  where for a particular wave function it was always the lowest power (0 or 1) of  $\sinh z$  which had the coefficient 1 multiplying it. In the RM discussion for  $a=0$ , the wave function is the hypergeometric function (3.8) expressed as a power series in  $u$ , multiplied by  $\cosh^{s-n} z$ . When one looks carefully, one finds that if the RM discussion is reexpressed as a power series in  $\sinh$  it is always the  $\sinh^n$  term which has  $\pm 1$  as the coefficient multiplying it. [The simplest way of noting this is that in the expansions of Eqs. (3.5) and (3.8), when  $a=0$ , the  $j=0$  term is the only contributor to  $e^{-nz} \cosh^{-s} z$ , this being needed for  $(\sinh z)^n / (\cosh z)^s$ . When one

takes account of the numerical factors, the coefficient reduces to  $\pm 1$ .] This all means that one should have

$$\alpha N_{\text{RM}}^{-2}(n) \Big|_{a=0} = \begin{cases} \frac{\alpha N_E^{-2}(n)}{A^2(\frac{1}{2}n, n, s)}, & n \text{ even} \\ \frac{\alpha N_O^{-2}(n)}{C^2(\frac{1}{2}(n-1), n, s)}, & n \text{ odd.} \end{cases} \quad (3.18a) \quad (3.18b)$$

Putting Eqs. (2.9) and (2.15) into Eq. (3.18a) and Eqs. (2.11) and (2.16) into Eq. (3.18b) one finds that both of them agree, as functions of  $n$ , with Eq. (3.17).

#### C. Morse and Feshbach formulation

A slightly different formulation of the problem is contained in Morse and Feshbach<sup>12</sup> (MF). There the minimum of the potential is centered at the origin, so that the potential is given by

$$V = V_0 \cosh^2 \mu [\tanh(\alpha x - \mu) + \tanh \mu]^2. \quad (3.19)$$

Comparing (1.2) with (3.19) one finds with a little algebra that to go from the MF problem to the RM problem one makes the transformation

$$V(x) = -\frac{B_0^2}{4V_0} + V \left( X = x + \frac{\mu}{\alpha}, \tanh \mu = \frac{B_0}{2U_0}, \right. \\ \left. V_0 = U_0 \left[ 1 - \left( \frac{B_0}{2U_0} \right)^2 \right] \right), \quad (3.20)$$

or

$$U_0 = V_0 \cosh^2 \mu, \quad B_0 = 2V_0 \cosh \mu \sinh \mu. \quad (3.21)$$

## IV. MATHEMATICAL DISCUSSION

### A. Jacobi and Gegenbauer polynomials, and associated Legendre functions

Our results (2.15), (2.16), and (3.15) and (3.16) for  $\alpha N_E^{-2}$ ,  $\alpha N_O^{-2}$ , and  $\alpha N_{\text{RM}}^{-2}$ , respectively, are given for the wave functions in terms of hypergeometric functions as described in Eqs. (2.6) combined with (2.2), (2.7) combined with (2.2), and (3.5) combined with (3.8), respectively. However, to obtain the closed-form normalizations, as an intermediate step we reexpressed the hypergeometric functions in terms of Jacobi polynomials in Eqs. (2.18), (2.23), and (3.12), respectively. Thus, if one wanted one could write the entire original wave functions in terms of these Jacobi polynomial formulas, and then the normalization constant expressions from (2.15), (2.16), and (3.15) and (3.16) for  $N_{E, O, \text{RM}}$  would be multiplied by the factors

$$\frac{1}{2}(n+1)B(\frac{1}{2}n+1, \frac{1}{2}), \quad (\frac{1}{2}n+1)B(\frac{1}{2}(n+1), \frac{3}{2}), \\ (s+a+1)B(n+1, s-n+a+1), \quad (4.1)$$

respectively. For Sec. IV B we observe that the RM solution can thus specifically be written

$$\begin{aligned}\psi_{\text{RM}} &= N_{\text{RM}J}(n) \frac{e^{az}}{\cosh^{s-n}z} P_n^{(s-n+a, s-n-a)}(-\tanh z) \\ &= (-1)^n N_{\text{RM}J}(n) (1 + \tanh z)^{(s-n+a)/2} (1 - \tanh z)^{(s-n-a)/2} P_n^{(s-n-a, s-n+a)}(\tanh z),\end{aligned}\quad (4.2)$$

$$N_{\text{RM}J}(n) = 2^{n-s} \left( \frac{\alpha(s-n+a)(s-n-a)\Gamma(2s-n+1)\Gamma(n+1)}{(s-n)\Gamma(s-a+1)\Gamma(s+a+1)} \right)^{1/2}. \quad (4.3)$$

Of course, given the functional form of (4.2),  $N_{\text{RM}J}(n)$  can now be directly verified as was done with Eqs. (3.13) and (3.14).

Further, for the  $B_0 = 0$  symmetric case (which means  $a = 0$  for the RM discussion), the Jacobi polynomials in the wave functions turn out to be three special cases which reduce to Gegenbauer polynomials. In particular, from Eqs. (22.5.25)–(22.5.27) of AS,<sup>16</sup> one has that

$$\begin{aligned}P_{n/2}^{(s-n, -1/2)}(2 \tanh^2 z - 1) &= \left[ \frac{\Gamma(s-n+\frac{1}{2})\Gamma(n+1)}{\Gamma(s-\frac{1}{2}n+\frac{1}{2})\Gamma(\frac{1}{2}n+\frac{1}{2})2^n} \right] \\ &\times C_n^{(s-n+1/2)}(\tanh z),\end{aligned}\quad (4.4)$$

$$\begin{aligned}P_{(n-1)/2}^{(s-n, +1/2)}(2 \tanh^2 z - 1) &= \left[ \frac{\Gamma(s-n+\frac{1}{2})\Gamma(n+1)}{\Gamma(s-\frac{1}{2}n+\frac{1}{2})\Gamma(\frac{1}{2}n+\frac{1}{2})2^n} \right] \\ &\times \tanh^{-1} z C_n^{(s-n+1/2)}(\tanh z),\end{aligned}\quad (4.5)$$

$$\begin{aligned}P_n^{(s-n, s-n)}(1-2u) &= P_n^{(s-n, s-n)}(-\tanh z) \\ &= (-1)^n P_n^{(s-n, s-n)}(\tanh z) \\ &= (-1)^n \left[ \frac{\Gamma(2s-2n+1)\Gamma(s+1)}{\Gamma(s-n+1)\Gamma(2s-n+1)} \right] \\ &\times C_n^{(s-n+1/2)}(\tanh z).\end{aligned}\quad (4.6)$$

So  $N_E$  and  $N_O$  obtained from wave functions described by the Gegenbauer polynomials in (4.4) and (4.5) would contain the further multiplicative factors of the quantities in the square brackets of (4.4) and (4.5), respectively. Similarly, if one wishes to express the wave functions for the symmetric case ( $a = 0$ ) of the RM formulation in terms of the Gegenbauer polynomials of Eq. (4.6), then the formula (4.3) for  $N_{\text{RM}J}(n)$  is multiplied by the quantity in the square brackets of (4.6) and then evaluated for  $a = 0$  which gives the normalization constant  $N_{\text{RM}J|_{a=0}}(n)$ . One now finds all the solutions are identical up to phases.<sup>14</sup>

But in this symmetric case there is one further transformation which gives the solutions in a particularly simple form. By observing from Eq. (22.5.60) of AS<sup>16</sup> that the Gegenbauer polynomials in (4.4)–(4.6) can be given as associated Legendre functions,

$$\begin{aligned}C_n^{(s-n+1/2)}(\tanh z) &= \frac{\Gamma(s-n+1)\Gamma(2s-n+1)}{\Gamma(n+1)\Gamma(2s-2n+1)} \\ &\times \left( \frac{-1}{2 \cosh z} \right)^{n-s} P_s^{(n-s)}(\tanh z),\end{aligned}\quad (4.7)$$

one finds that  $\psi_E$ ,  $\psi_O$ , and  $\psi_{\text{RM}}|_{a=0}$  all have the final normalized solution

$$\begin{aligned}\psi_{E, O, \text{RM}}|_{a=0} &= \phi_{E, O, \text{RM}}|_{a=0} \left[ \frac{\alpha(s-n)\Gamma(2s-n+1)}{\Gamma(n+1)} \right]^{1/2} \\ &\times P_s^{(n-s)}(\tanh z),\end{aligned}\quad (4.8)$$

where the  $\phi$  are the unimportant phase factors  $(-1)^{-s/2}$ ,  $(-1)^{-(s-1)/2}$ , and  $(-1)^{-(s+n)/2}$ . Again, given the functional form of the solution (4.8), the normalization constant can be simply verified by using Eq. (7.122.3) of GR.<sup>17</sup>

The results we have obtained are gathered in Appendix B.

By adding a zero point energy  $+U_0$  to the system, and then taking the limits  $\alpha \rightarrow 0$ ,  $s \rightarrow \infty$ , but such that  $\alpha^2 s = m\omega/\hbar$ , one can show, with the aid of the standard formula relating the limit of Gegenbauer polynomials to Hermite polynomials, that the normalized wave functions (B17) for this symmetric case go over exactly to the normalized wave functions for the simple harmonic oscillator, as do the energy levels and potential.

## B. Connection to Riemann's equation

Given the especially simple solutions of Eqs. (4.2) and (4.8) one might expect that one could be able to obtain them directly, instead of via a series of transformations on the standard LL and RM solutions. Indeed, as Simmons has kindly pointed out to me, this is indeed the case. By changing variables in Eqs. (1.1) and (1.2) to  $g = \tanh \alpha x$ , one obtains

$$\begin{aligned}\left( (1-g^2)^2 \frac{\partial^2}{\partial g^2} - 2g(1-g^2) \frac{\partial}{\partial g} \right. \\ \left. - v_1 g + v_0(1-g^2) - \epsilon \right) \psi = 0,\end{aligned}\quad (4.9)$$

$$(v_1, v_0, \epsilon) = \frac{2m}{\hbar^2 \alpha^2} (B_0, U_0, -E). \quad (4.10)$$

Equation (4.9) is of the form of Riemann's  $P$  equation. (See Sec. 15.6 of AS.<sup>16</sup>) It has singularities at  $g = (-1, 1, \infty)$  and exponents, in the standard notation  $(\alpha, \alpha'; \beta, \beta'; \gamma, \gamma')$ , of

$$\begin{aligned} -\alpha' = \alpha = \frac{1}{2}(\epsilon - v_1)^{1/2}, \quad -\beta' = \beta = \frac{1}{2}(\epsilon - v_1)^{1/2}, \\ 1 - \gamma' = \gamma = 1 + s. \end{aligned} \quad (4.11)$$

(The reader should not confuse the exponents with the other notation we have used.) For the solutions which vanish at  $g = -1$  the Riemann  $P$  symbol can be reduced to a hypergeometric function which is a Jacobi polynomial in  $\frac{1}{2}(g+1)$  with the factors  $(g+1)^\alpha(g-1)^\beta$  extracted. This is the functional form of the complete solution (4.2).

For the symmetric case, things are even more direct. For  $v_1 = 0$  in (4.9), the Riemann equation is the Legendre equation. The solution which vanishes at  $g = \pm 1$  is the Legendre function  $P_s^{(n-s)}(g)$ , which is the functional form of the solution (4.8).

### C. Relation to the factorization method

In their classic paper on Schrödinger's<sup>23</sup> factorization method, Infeld and Hull<sup>15</sup> described how exactly solvable second-order potential problems with boundary conditions can be factorized into two first-order differential equations from which the eigenvalues and normalized eigenfunctions can be generated. Intuitively one can see that this method is describing an equation as a product of a raising and a lowering operator, since these first-order differential equations are combinations of a derivative and a function of  $x$ , as in the harmonic oscillator<sup>24</sup>  $[a^+ = (a^-)^\dagger]$

$$a^- = [i/(2m\hbar\omega)^{1/2}](p - im\omega x). \quad (4.12)$$

Infeld and Hull applied their method to the RM problem with the complete potential of Eq. (1.2). Their results, in our notation of Sec. III, were that the normalized wave functions could be generated, one by one, by the procedure<sup>25</sup>

$$\Psi_n = \Theta_n^n \Phi_n, \quad (4.13)$$

$$\begin{aligned} \Phi_n = \left( \frac{2^{1-2s+2n} \alpha \Gamma(2s-2n)}{\Gamma(s-n-a)\Gamma(s-n+a)} \right)^{1/2} \\ \times (\cosh^{-s+n} \alpha x) e^{\alpha x}, \end{aligned} \quad (4.14)$$

$$\begin{aligned} \Theta_n = \left[ \alpha^2 n(s-n) \left( 1 - \frac{1}{s^2} \right) \right]^{-1/2} \\ \times \left( s \alpha \tanh \alpha x - \frac{\alpha a(s-n)}{s} - \frac{\partial}{\partial x} \right), \end{aligned} \quad (4.15)$$

where  $s$  and  $a(n)$  remain as defined in Eqs. (3.6) and (3.7). We have verified for the first two cases ( $n=0$  and  $n=1$ ) that Eqs. (4.13)–(4.15) agree exactly with the wave function (3.5) when  $F$  is given by the power series (3.8) and  $N_{RM}$  is as we obtained

in Eqs. (3.15) and (3.16).

Note, however, that the Infeld-Hull factorization of this problem is important as a matter of principle rather than of practicality for molecular problems. This is because if one takes typical molecular characteristics, the number of bound states  $N$  is (for the symmetric problem)

$$N = 1 + n_{\max} = 1 + [s], \quad (4.16)$$

$$s \approx 21.9 \delta^{1/2} \mathfrak{M}^{1/2} \alpha - \frac{1}{2}, \quad (4.17)$$

where  $\delta$  is  $U_0$  in eV,  $\mathfrak{M}$  is the reduced mass  $m$  in a.m.u., and  $\alpha$  is  $1/\alpha$  in Å. Thus, there will be many tens of bound states in a typical molecular-model problem. This is far too many states to generate all  $N$  of the  $\Psi_n$  by using  $N$  different  $\Theta_n$ , each to be applied  $n$  times to the  $N$  separate  $\Phi_n$ . The closed-form expressions (4.2) and (4.8) for arbitrary  $n$  are clearly preferable to the above procedure.<sup>14</sup>

### V. DISCUSSION

Much work has been done on the connection of the special functions of mathematical physics to group theory.<sup>26</sup> Indeed, as we alluded to in Sec. IV, the factorization method, with its raising and lowering operator structure, is a classic study of this type. The most familiar example is the harmonic oscillator. Its eigenfunctions are Hermite polynomials and its group structure is  $SU(1,1)$ . Also, the important coherent states of the harmonic oscillator are eigenfunctions of the destruction operator of Eq. (4.12):

$$a |\alpha\rangle = \alpha |\alpha\rangle, \quad |\alpha\rangle = \exp(-|\alpha|^2) \sum_{n=0}^{\infty} \frac{\alpha^n}{(n!)^{1/2}} |n\rangle. \quad (5.1)$$

These coherent states of the harmonic oscillator are extremely useful calculational tools. For example, if one considers the forced harmonic oscillator with the external forcing function  $F(t)$ , arbitrary, one can solve the transition probabilities exactly. However, if one does this calculation entirely with number states the calculation is quite involved.<sup>27,28</sup> On the other hand, with the use of coherent states the calculation is surprisingly simple.<sup>24</sup>

It is important to consider our potential in the light of the above. The RM potential is a useful model of molecules. With our results one now has the number-state wave functions complete with normalizations. One can therefore ask what the coherent states of this system are. In principle they exist and can be found by function or group theory techniques. They should also be able to be expressed in terms of continuum states and the normed number states we now have. Finally, with the coherent states of this system in hand, one

could discuss the forced-oscillator problem. Perhaps with the coherent states of this system the forced-oscillator problem would be more tractable to analytic techniques, as is the case with the forced harmonic oscillator. Such a discussion could serve as an analytic model calculation of the excitation and dissociation of molecules by laser light.<sup>29,30</sup>

The coherent states for this system will be discussed elsewhere.<sup>31</sup>

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#### APPENDIX A: SYMMETRIC-CASE WAVE FUNCTIONS UP TO $n = 8$

Given that the symmetric-case wave functions are

$$\psi(n) = \frac{N(n) \omega(n)}{(\cosh z)^s}, \quad z \equiv \alpha x, \quad (\text{A1})$$

we explicitly write below the even- and odd-wave-function quantities  $N(n) \omega(n)$  up to  $n = 8$ . First the even quantities:

$$N_E(0) \omega_E(0) = \left( \frac{\alpha}{B(\frac{1}{2}, s)} \right)^{1/2}, \quad (\text{A2})$$

$$N_E(2) \omega_E(2) = \left( \frac{\alpha}{B(\frac{1}{2}, s)} \frac{(s-2)}{(2s-1)} \right)^{1/2} [1 - 2(s-1) \sinh^2 z], \quad (\text{A3})$$

$$N_E(4) \omega_E(4) = \left( \frac{\alpha}{B(\frac{1}{2}, s)} \frac{3}{2} \frac{(s-1)(s-4)}{(2s-1)(2s-3)} \right)^{1/2} [1 - 4(s-2) \sinh^2 z + \frac{4}{3}(s-2)(s-3) \sinh^4 z], \quad (\text{A4})$$

$$N_E(6) \omega_E(6) = \left( \frac{\alpha}{B(\frac{1}{2}, s)} \frac{5}{2} \frac{(s-1)(s-2)(s-6)}{(2s-1)(2s-3)(2s-5)} \right)^{1/2} \times [1 - 6(s-3) \sinh^2 z + 4(s-3)(s-4) \sinh^4 z - \frac{8}{15}(s-3)(s-4)(s-5) \sinh^6 z], \quad (\text{A5})$$

$$N_E(8) \omega_E(8) = \left( \frac{\alpha}{B(\frac{1}{2}, s)} \frac{5}{4} \frac{7}{2} \frac{(s-1)(s-2)(s-3)(s-8)}{(2s-1)(2s-3)(2s-5)(2s-7)} \right)^{1/2} \times [1 - 8(s-4) \sinh^2 z + 8(s-4)(s-5) \sinh^4 z - \frac{48}{15}(s-4)(s-5)(s-6) \sinh^6 z + (16/7!!)(s-4)(s-5)(s-6)(s-7) \sinh^8 z]. \quad (\text{A6})$$

Next the odd quantities:

$$N_O(1) \omega_O(0) = \left( \frac{\alpha}{B(\frac{3}{2}, s-1)} \right)^{1/2} \sinh z \quad (\text{A7})$$

$$N_O(3) \omega_O(3) = \left( \frac{\alpha}{B(\frac{3}{2}, s-1)} \frac{3(s-3)}{(2s-1)} \right)^{1/2} \sinh z [1 - \frac{2}{3}(s-2) \sinh^2 z] \quad (\text{A8})$$

$$N_O(5) \omega_O(5) = \left( \frac{\alpha}{B(\frac{3}{2}, s-1)} \frac{(3)(5)}{2} \frac{(s-2)(s-5)}{(2s-1)(2s-3)} \right)^{1/2} \sinh z [1 - \frac{4}{3}(s-3) \sinh^2 z + \frac{4}{15}(s-3)(s-4) \sinh^4 z], \quad (\text{A9})$$

$$N_O(7) \omega_O(7) = \left( \frac{\alpha}{B(\frac{3}{2}, s-1)} \frac{(5)(7)}{2} \frac{(s-2)(s-3)(s-7)}{(2s-1)(2s-3)(2s-5)} \right)^{1/2} \times \sinh z [1 - 2(s-4) \sinh^2 z + \frac{4}{5}(s-4)(s-5) \sinh^4 z - (8/7!!)(s-4)(s-5)(s-6) \sinh^6 z]. \quad (\text{A10})$$





When the symmetric-case normalization constants are written in terms of Gegenbauer polynomials or Legendre functions, both the RM and LL formulations collapse into the same formulas, specifically

$$\psi_G = 2^{s-n} \Gamma(s-n+\frac{1}{2}) \left( \frac{\alpha(s-n)\Gamma(n+1)}{\pi\Gamma(2s-n+1)} \right)^{1/2} \times \cosh^{n-s} z C_n^{(s-n+1/2)}(\tanh z), \quad (\text{B17})$$

$$\psi_L = \left( \frac{\alpha(s-n)\Gamma(2s-n+1)}{\Gamma(n+1)} \right)^{1/2} P_s^{(n-s)}(\tanh z). \quad (\text{B18})$$

### Three-dimensional case

For the  $l=0$  S-wave case, the problem is solvable in three dimensions as indicated in Sec. II B. Only the odd solutions of the one-dimensional case remain and one has

$$\psi_{\rho,00}(r) = \sqrt{2} r^{-1} \psi_{LL0}(z = \alpha x - \alpha r, n = 2\rho + 1) (4\pi)^{-1/2}, \quad \rho = 0, 1, 2, \dots \quad (\text{B19})$$

$$\psi = [2\alpha(\kappa + \lambda + 2n)\Gamma(n+1)\Gamma(\kappa + \lambda + n)\Gamma(\kappa + n + \frac{1}{2})/\Gamma(\lambda + n + \frac{1}{2})]^{1/2} \times [\Gamma(\kappa + \frac{1}{2})\Gamma(\lambda + \frac{1}{2})]^{-1} (\sin z)^\kappa (\cos z)^\lambda F(-n, \kappa + \lambda + n; \kappa + \frac{1}{2}; \sin^2 z) \quad (\text{C3})$$

$$= \left( \frac{2\alpha(\kappa + \lambda + 2n)\Gamma(n+1)\Gamma(\kappa + \lambda + n)}{\Gamma(\kappa + n + \frac{1}{2})\Gamma(\lambda + n + \frac{1}{2})} \right)^{1/2} (\sin z)^\kappa (\cos z)^\lambda P_n^{(\kappa-1/2, \lambda-1/2)}(1 - 2\sin^2 z). \quad (\text{C4})$$

For the symmetric case ( $\kappa = \lambda$ ) one further has that

$$\psi = \frac{2\Gamma(2\lambda)}{\Gamma(\lambda + \frac{1}{2})} \left( \frac{\alpha(\lambda + n)\Gamma(n+1)}{\Gamma(2\lambda + n)} \right)^{1/2} (\sin z \cos z)^\lambda \times C_n^{(\lambda)}(1 - 2\sin^2 z) \quad (\text{C5})$$

$$= \left( \frac{4\alpha(\lambda + n)\Gamma(2\lambda + n)}{\Gamma(n+1)} \right)^{1/2} (\sin z \cos z)^{\lambda/2} \times P_{n+\lambda-1/2}^{(1/2-\lambda)}(1 - 2\sin^2 z). \quad (\text{C6})$$

In this symmetric case it actually is preferable to make a change to the variable  $\bar{z} \equiv \alpha \bar{x} = 2\alpha x - \frac{1}{2}\pi$ , which means that the potential and energy levels are given by  $(-\frac{1}{2}\pi \leq \bar{z} \leq \frac{1}{2}\pi)$

$$V(\bar{x}) = \frac{\hbar^2 \alpha^2}{2m} \frac{\lambda(\lambda-1)}{\cos^2 \bar{z}}, \quad E_n = \frac{\hbar^2 \alpha^2}{2m} (\lambda + n)^2, \quad (\text{C7})$$

and the normalized wave functions are

### APPENDIX C: NORMALIZATION CONSTANTS FOR THE PÖSCHL-TELLER POTENTIAL

A potential which is mathematically related to the  $\cosh^{-2}$  potential is the Pöschl-Teller potential,<sup>32-34</sup>

$$V(x) = \frac{\hbar^2 \alpha^2}{2m} \left( \frac{\kappa(\kappa-1)}{\sin^2 \alpha x} + \frac{\lambda(\lambda-1)}{\cos^2 \alpha x} \right), \quad \kappa, \lambda > 1, \quad (\text{C1})$$

whose Schrödinger equation eigenvalues are

$$E_n = \frac{\hbar^2 \alpha^2}{2m} (\kappa + \lambda + 2n)^2, \quad n = 0, 1, 2, \dots \quad (\text{C2})$$

This potential is periodic. However, each period is separated from the next by an infinite potential barrier so it can be studied within one period, say  $0 \leq z \equiv \alpha x \leq \frac{1}{2}\pi$ . The potential is asymmetric about  $z = \frac{1}{4}\pi$  (unless  $\kappa = \lambda$ ), and the minimum of the well is located at  $z_{\min} \cong \frac{1}{4}\pi$  as  $\kappa \geq \lambda$ . By the same techniques as used in the main part of this paper, one has that the exact, normalized wave functions can be given as (we ignore phase factors below)

$$\psi(\bar{x}) = \left( \frac{\alpha(\lambda + n)\Gamma(2\lambda + n)}{\Gamma(n+1)} \right)^{1/2} (\cos \bar{z})^{\lambda/2} \times P_{n+\lambda-1/2}^{(1/2-\lambda)}(\sin \bar{z}). \quad (\text{C8})$$

It is interesting to observe that for (C7) and (C8) as  $\lambda \rightarrow 1$ , the potential, energy levels, and normalized wave functions become exactly those for the infinite square well potential with barriers at  $\bar{x} = \pm\pi/2\alpha \equiv \pm a$ , in terms of the number  $N = n + 1$ . Also, by first subtracting the zero point energy  $\lambda(\lambda-1)\hbar^2\alpha^2/2m$  and then taking the limits  $\lambda \rightarrow \infty$ ,  $\alpha \rightarrow 0$ , but such that  $\alpha^2\lambda = m\omega/\hbar$ , one can show that the potential, energy levels, and normalized wave functions become those for the simple harmonic oscillator. This can be done in the same manner as mentioned at the end of Sec. IV A for the similar limits of the  $\cosh^{-2}$  potential.

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