The nonrelativistic oscillator strength of a hyperbolic-type potential

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We consider the D-dimensional Schrödinger equation under the hyperbolic potential $V_0(1-\coth(\alpha r))+V_1(1-\coth(\alpha r))^2$. Using a Pekeris-type approximation, the approximate analytical solutions of the problem are obtained via the supersymmetric quantum mechanics. The behaviors of energy eigenvalues versus dimension are discussed for various quantum numbers. Useful expectation values as well as the oscillator strength are obtained.

Keywords: Schrödinger equation, D-dimensional space, hyperbolic potential, supersymmetry quantum mechanics, oscillator strength

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1. Introduction

Although a few physical potentials are analytically solvable, there exist many potentials for which approximate schemes are inevitable.[1] Amongst such potentials, the hyperbolic ones are appealing cases of study in either relativistic or nonrelativistic regimes.[2–20] They have been used in the study of nuclear shell models, distribution of nuclear densities, and elastic scattering.[21–24] Investigation of metallic clusters and optical models has also performed on the basis of these interactions.[25,26] In the present work, for the sake of generality, we study the D-dimensional Schrödinger equation for the hyperbolic potential

$$V_0(1-\coth(\alpha r))+V_1(1-\coth(\alpha r))^2, \tag{1}$$

which resembles the Kratzer potential for small r and vanishes for large r.

2. The supersymmetric quantum mechanics (SUSYQM)

To preserve the continuity, we review the SUSYQM in a few lines. Now we consider the so-called partner Hamiltonians[27,28]

$$H_\pm = \frac{p^2}{2m}+V_\pm(x), \tag{2}$$

where

$$V_\pm(x) = \Phi^2(x)\pm\Phi'(x). \tag{3}$$

If we assume a good supersymmetry (SUSY), i.e., $E_0=0$, the ground state of the system is obtained via

$$\phi_0^-(x) = C\,\mathrm{e}^{-U(x)}, \tag{4}$$

where C is a normalization constant and

$$U(x) = \int_{x_0}^{x}\mathrm{d}x\Phi(x). \tag{5}$$

If the condition

$$V_+(a_0,x) = V_-(a_1,x)+R(a_1) \tag{6}$$

holds, the partner Hamiltonians are called shape-invariant. In Eq. (6) a_1 is a new set of parameters uniquely determined from the old set a_0 via the mapping $F: a_0\mapsto a_1=F(a_0)$ and $R(a_1)$ does not include x. In the presence of shape-invariance, the eigenvalues and the eigenfunctions are obtained via[27,28]

$$E_n = \sum_{s=1}^{n}R(a_s), \tag{7a}$$

$$\phi_n^-(a_0,x) = \prod_{s=0}^{n-1}\Big[\frac{A^\dagger(a_s)}{[E_n-E_s]^{1/2}}\Big]\phi_0^-(a_n,x), \tag{7b}$$

$$\phi_0^-(a_n,x) = C\exp\Big\{-\int_0^x\mathrm{d}x\Phi(a_n,x)\Big\}, \tag{7c}$$

with

$$A_s^\dagger = -\frac{\partial}{\partial x}+\Phi(a_s,x). \tag{8}$$

In fact, we obtain the spectrum of the following Hamiltonian

$$H_s = -\frac{\partial^2}{\partial x^2}+V_-(a_s,x)+E_s, \tag{9}$$

which satisfies the following eigenvalue equation

$$H_s\phi_{n-s}^-(a_s,x) = E_n\phi_{n-s}^-(a_s,x), \quad n\geq s \tag{10}$$

with

$$\phi_{n-s}^-(a_s,x) = \frac{A^\dagger}{[E_n-E_s]^{1/2}}\phi_{n-(s+1)}^-(a_{s+1},x). \tag{11}$$

After the removal of the angle part, the radial Schrödinger equation is obtained as[29,30]

$$\Big[\frac{\mathrm{d}^2}{\mathrm{d}r^2}+\frac{D-1}{r}\frac{\mathrm{d}}{\mathrm{d}r}+\frac{2\mu}{\hbar^2}(E_{n,l}^D-V(r))-\frac{l(l+D-2)}{r^2}\Big]R_{n,l}(r) = 0, \quad 0\leq r\leq\infty, \tag{12}$$

where l denotes the angular momentum quantum number. To remove the first-order derivative, we apply the well-known transformation

$$u_{n,l}(r) = r^{(D-1)/2}R_{n,l}(r), \tag{13}$$

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which results in

$$\Big[\frac{\mathrm{d}^2}{\mathrm{d}r^2}-\frac{(D+2l-1)(D+2l-3)}{4r^2}-\frac{2m}{\hbar^2}V_0(1-\coth(\alpha r))$$
$$-\frac{2m}{\hbar^2}V_1(1-\coth(\alpha r))^2+\frac{2m}{\hbar^2}E^D_{n,l}\Big]u_{n,l}(r)=0, \quad (14)$$

where V_0 and V_1 can be arbitrary numbers. By using the following approximation

$$\frac{1}{r^2}\sim\frac{\alpha^2}{\sinh^2(\alpha r)}=\alpha^2(\coth^2(\alpha r)-1), \quad (15)$$

we have

$$\Big[\frac{\mathrm{d}^2}{\mathrm{d}r^2}-\frac{\alpha^2(D+2l-1)(D+2l-3)}{4}[\coth^2(\alpha r)-1]$$
$$-\frac{2mV_0}{\hbar^2}(1-\coth(\alpha r))-\frac{2mV_1}{\hbar^2}(1-\coth(\alpha r))^2$$
$$+\frac{2mE^D_{n,l}}{\hbar^2}\Big]u_{n,l}(r)=0, \quad (16)$$

or equivalently

$$\Big[\frac{\mathrm{d}^2}{\mathrm{d}r^2}+\Big\{-\frac{\alpha^2(D+2l-1)(D+2l-3)}{4}-\frac{2mV_1}{\hbar^2}\Big\}\mathrm{csch}^2(\alpha r)$$
$$+\Big\{\frac{2mV_0}{\hbar^2}+\frac{4mV_1}{\hbar^2}\Big\}\coth(\alpha r)$$
$$+\Big\{-\frac{2mV_0}{\hbar^2}-\frac{4mV_1}{\hbar^2}+\frac{2mE^D_{n,l}}{\hbar^2}\Big\}\Big]u_{n,l}(r)=0, \quad (17)$$

which may be written more neatly as

$$-\frac{\mathrm{d}^2u_{n,l}(r)}{\mathrm{d}r^2}+V_{\mathrm{eff}}(r)u_{n,l}(r)=\tilde{E}_{n,l}u_{n,l}(r), \quad (18)\ (18)$$

with

$$V_{\mathrm{eff}}(r)=-V_1'\,\mathrm{csch}^2(\alpha r)-V_2'\coth(\alpha r), \quad (19a)$$
$$\tilde{E}_{n,l}=-\frac{2mV_0}{\hbar^2}-\frac{4mV_1}{\hbar^2}+\frac{2m\mathrm{E}^D_{n,l}}{\hbar^2}, \quad (19b)$$

where

$$V_1'=-\frac{\alpha^2(D+2l-1)(D+2l-3)}{4}-\frac{2mV_1}{\hbar^2}, \quad (20a)$$
$$V_2'=\frac{2mV_0}{\hbar^2}+\frac{4mV_1}{\hbar^2}. \quad (20b)$$

The ground state (GS) can be determined from the following Riccati equation

$$\phi^2-\phi'=V_{\mathrm{eff}}-\tilde{E}_{0,l}, \quad (21)$$

whose solution is

$$\phi(r)=A+B\coth(\alpha r). \quad (22)$$

Therefore, from Eqs. (4) and (5), the GS wavefunction is

$$u_{0,l}(r)=\exp\Big(-\int\phi(r)\,\mathrm{d}r\Big), \quad (23)$$

or

$$u_{0,l}(r)=\exp(Ar)\sinh^{B/\alpha}(\alpha r). \quad (24)$$

Substituting Eq. (22) into Eq. (21) and comparing equal powers we can find

$$2BA=-V_2', \quad (25a)$$
$$B^2+\alpha B=-V_1', \quad (25b)$$
$$(A^2+B^2)=-\tilde{E}_{0,l}, \quad (25c)$$

or equivalently

$$A=-\frac{V_2'}{2B}, \quad (26a)$$
$$B=\frac{1}{2}\Big[-\alpha\pm\sqrt{\alpha^2-4V_1'}\Big], \quad (26b)$$
$$\tilde{E}_{0,l}=-(A^2+B^2)=-\Big(\frac{V_2'^2}{4B^2}+B^2\Big). \quad (26c)$$

Now we construct the partner potentials

$$V_{\mathrm{eff}+}(r)=\phi^2+\frac{\mathrm{d}\phi}{\mathrm{d}r}$$
$$=\mathrm{csch}^2(\alpha r)[B^2-\alpha B]+B^2+\frac{V_2'^2}{4B^2}-V_2'\coth(\alpha r), \quad (27a)$$
$$V_{\mathrm{eff}-}(r)=\phi^2-\frac{\mathrm{d}\phi}{\mathrm{d}r}$$
$$=\mathrm{csch}^2(\alpha r)[B^2+\alpha B]+B^2+\frac{V_2'^2}{4B^2}-V_2'\coth(\alpha r), \quad (27b)$$

which satisfy the shape-invariant condition

$$V_{\mathrm{eff}+}(r,a_0)=V_{\mathrm{eff}-}(r,a_1)+R(a_1), \quad (28)$$

via the mapping $B\to B+\alpha$. The corresponding reminders are

$$R(a_1)=\Big(\frac{V_2'^2}{4a_0^2}+a_0^2\Big)-\Big(\frac{V_2'^2}{4a_1^2}+a_1^2\Big),$$
$$R(a_2)=\Big(\frac{V_2'^2}{4a_1^2}+a_1^2\Big)-\Big(\frac{V_2'^2}{4a_2^2}+a_2^2\Big),$$
$$\vdots$$
$$R(a_n)=\Big(\frac{V_2'^2}{4a_{n-1}^2}+a_{n-1}^2\Big)-\Big(\frac{V_2'^2}{4a_n^2}+a_n^2\Big),$$
$$\tilde{E}^-_{n,l}=\sum_{k=1}^{n}R(a_k)=\Big(\frac{V_2'^2}{4a_0^2}+a_0^2\Big)-\Big(\frac{V_2'^2}{4a_n^2}+a_n^2\Big), \quad (29)$$

where $n=0,1,2,\ldots$ and

$$a_n=a_0-n\alpha. \quad (30)$$

From Eqs. (25c) and (29) the eigenvalues can be found to be

$$\tilde{E}_{n,l}=\tilde{E}^-_{n,l}+\tilde{E}_{0,l}=-\Big(\frac{V_2'^2}{4a_n^2}+a_n^2\Big)$$
$$=-\Big(\frac{V_2'^2}{4(B-n\alpha)^2}+(B-n\alpha)^2\Big), \quad (31)$$

or, more neatly to be

$$E^D_{n,l}=-\frac{m(V_0+2V_1)^2}{2\hbar^2(B-n\alpha)^2}-\frac{\hbar^2}{2m}(B-n\alpha)^2+V_0+2V_1. \quad (32)$$

In order to obtain the wavefunction, we start from Eq. (17)

$$\Big[\frac{\mathrm{d}^2}{\mathrm{d}r^2}+\Big\{-\frac{\alpha^2(D+2l-1)(D+2l-3)}{4}-\frac{2mV_1}{\hbar^2}\Big\}\mathrm{csch}^2(\alpha r)$$
$$+\Big\{\frac{2mV_0}{\hbar^2}+\frac{4mV_1}{\hbar^2}\Big\}\coth(\alpha r)$$
$$+\Big\{-\frac{2mV_0}{\hbar^2}-\frac{4mV_1}{\hbar^2}+\frac{2mE_{n,l}}{\hbar^2}\Big\}\Big]u_{n,l}(r)=0, \quad (33)$$

which can be written as

$$z^2\frac{\mathrm{d}^2u_{n,l}(z)}{\mathrm{d}z^2}+z\frac{\mathrm{d}u_{n,l}(z)}{\mathrm{d}z}+\Big\{\Big(-\frac{V_1'}{\alpha^2}+\frac{V_2'}{4\alpha^2}\Big)\frac{1}{1-z}$$

$$+\frac{V_1'}{\alpha^2}\frac{1}{(1-z)^2}+\frac{V_2'}{4\alpha^2}\frac{z}{(1-z)}+\frac{V_3'}{4\alpha^2}\Big\}u_{n,l}(z)=0, \quad (34)$$

where

$$V_3'=-\frac{2mV_0}{\hbar^2}-\frac{4mV_1}{\hbar^2}+\frac{2mE_{n,l}}{\hbar^2}, \quad (35a)$$

$$z=\exp(-2\alpha r). \quad (35b)$$

Now, we analyze the asymptotic behavior of Eq. (34).[31] When $r\to 0$ ($z\to 1$), the solution is $u_{n,l}(z)=(1-z)^{\lambda}$ with

$$\lambda=l'+1, \quad (36a)$$

$$l'=\frac{1}{2}\Big(-1+\sqrt{1-\frac{4V_1'}{\alpha^2}}\Big). \quad (36b)$$

In the other limit, i.e. $r\to\infty$ ($z\to 0$), we have the solution $u_{n,l}(z)=z^{\eta}$ where

$$\eta=\sqrt{-\frac{V_2'+V_3'}{4\alpha^2}}. \quad (37)$$

Therefore, we use the transformation $u_{n,l}(z)=z^{\eta}(1-z)^{\lambda}f_{nl}(z)$ which brings Eq. (34) into the following form

$$(1-z)z\frac{\mathrm{d}^2 f_{nl}(z)}{\mathrm{d}z^2}+[1+2\eta-(1+2\lambda+2\eta)z]\frac{\mathrm{d}f_{nl}(z)}{\mathrm{d}z}$$
$$-\Big(2\lambda\eta+\eta^2+\lambda^2+\frac{V_3'}{4\alpha^2}-\frac{V_2'}{4\alpha^2}\Big)f_{nl}(z)=0. \quad (38)$$

The above equation is just a hypergeometric equation whose solutions are written in terms of the hypergeometric function

$$f_{nl}(z)={}_2\mathrm{F}_1(a,b;1+2\eta;z), \quad (39)$$

with

$$a=\lambda+\eta+\sqrt{-\frac{V_3'}{4\alpha^2}+\frac{V_2'}{4\alpha^2}}, \quad (40a)$$

$$b=\lambda+\eta-\sqrt{-\frac{V_3'}{4\alpha^2}+\frac{V_2'}{4\alpha^2}}. \quad (40b)$$

When either a or b is a negative integer, the hypergeometric function $f_{nl}(z)$ reduces to a polynomial of degree n. Therefore

$$\begin{aligned}f_{nl}(z)&={}_2\mathrm{F}_1(a,b;1+2\eta;z)\\&={}_2\mathrm{F}_1(-n,n+2\lambda+2\eta;1+2\eta;z)\\&={}_2\mathrm{F}_1\Big(-n,n+2(l'+1)+2\sqrt{-\frac{V_2'+V_3'}{4\alpha^2}};1\\&\quad+2\sqrt{-\frac{V_2'+V_3'}{4\alpha^2}};\exp(-2\alpha r)\Big). \quad (41)\end{aligned}$$

So, we have

$$\begin{aligned}u_{n,l}(z)&=z^{\eta}(1-z)^{\lambda}f_{nl}(z)\\&=N_{nl}\exp\Big(-2\alpha\sqrt{-\frac{V_2'+V_3'}{4\alpha^2}}r\Big)(1-\exp(-2\alpha r))^{l'+1}\\&\quad\times{}_2\mathrm{F}_1\Big(-n,n+2(l'+1)+2\sqrt{-\frac{V_2'+V_3'}{4\alpha^2}};1\\&\quad+2\sqrt{-\frac{V_2'+V_3'}{4\alpha^2}};\exp(-2\alpha r)\Big), \quad (42)\end{aligned}$$

with the normalization being

$$N_{nl}=\frac{\Gamma\Big(n+1+2\sqrt{-\frac{V_2'+V_3'}{4\alpha^2}}\Big)}{n!\Gamma\Big(1+2\sqrt{-\frac{V_2'+V_3'}{4\alpha^2}}\Big)}. \quad (43)$$

Figures 1–3 show the plots of $E_{n,l}$ versus α, V_0, and V_1 for various quantum numbers. The wavefunctions are depicted in Fig. 4 for different values of n, l, and s.

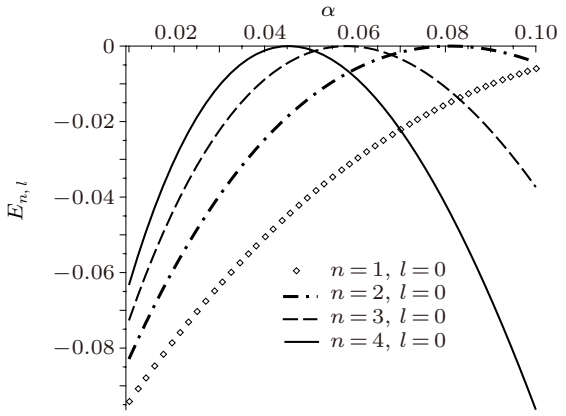


Fig. 1. Plots of $E_{n,l}$ versus α for $\hbar=1$, $m=1$, $V_0=0.3$, $V_1=0.2$, and $D=3$.

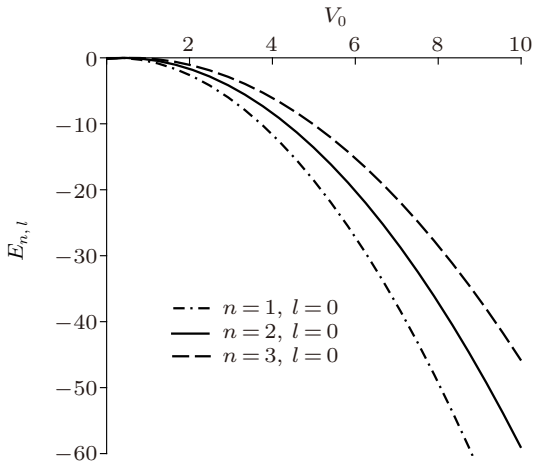


Fig. 2. Plots of $E_{n,l}$ versus V_0 for $\hbar=1$, $m=1$, $\alpha=0.1$, $V_1=0.2$, and $D=3$.

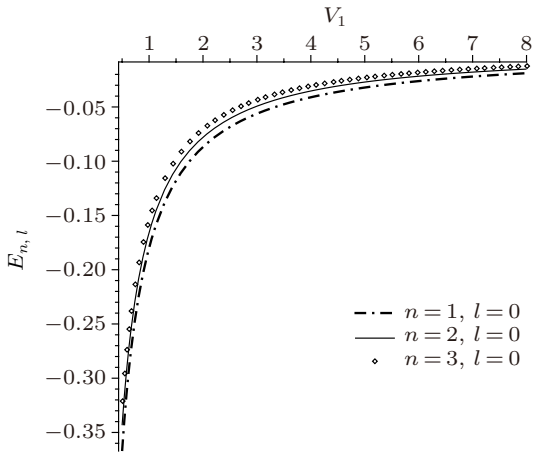


Fig. 3. Plots of $E_{n,l}$ versus V_1 for $\hbar=1$, $m=1$, $\alpha=0.01$, $V_0=0.9$, and $D=3$.

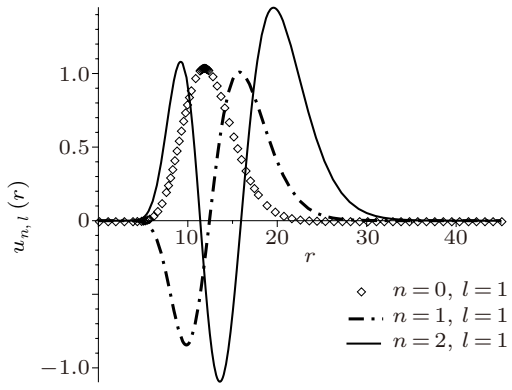


Fig. 4. Wavefunctions for some values of n and l.

3. Some useful physical quantities

3.1. Some expectation values for the hyperbolic potential in D dimensions

In many studies, we frequently need some expectation values which we calculate in this section using the Hellmann–Feynman theorem (HFT).[32,33] According to this theorem, if the Hamiltonian H of a system is a function of some parameter q, then the energy eigenvalue $E_{n,l}(q)$ and the eigenfunction $U_{n,l}(q)$ are related via the relation

$$\frac{\partial E_{n,l}(q)}{\partial q} = \langle U_{n,l}(q)|\frac{\partial H(q)}{\partial q}|U_{n,l}(q)\rangle. \tag{44}$$

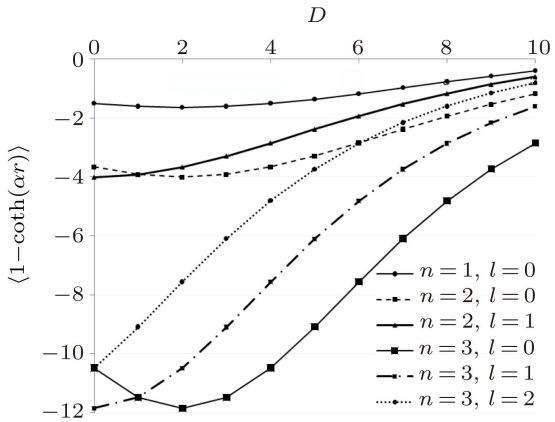


Fig. 5. Plots of $\langle 1-\coth(\alpha r)\rangle$ versus D.

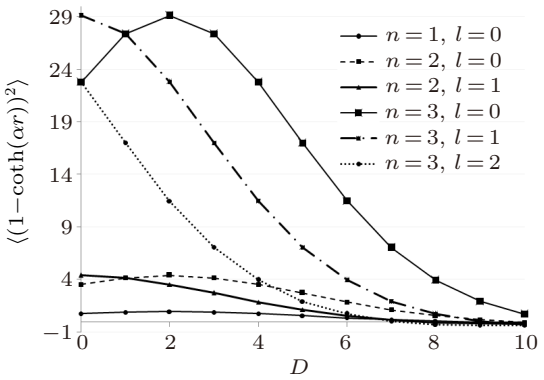


Fig. 6. Plots of $\langle(1-\coth(\alpha r))^2\rangle$ versus D.

In our study,

$$H = -\frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{\hbar^2}{2\mu}\frac{(D+2l-1)(D+2l-3)}{4r^2} + V_0(1-\coth(\alpha r)) + V_1(1-\coth(\alpha r))^2. \tag{45}$$

In order to calculate $\langle r^{-2}\rangle$, we set $q=l$ such that[34]

$$\frac{\partial E_{n,l}}{\partial l} = \langle U_{n,l}(l)\left|\frac{\partial H(l)}{\partial l}\right|U_{n,l}(l)\rangle = \frac{\hbar^2}{2\mu}(2l+D-2)\langle r^{-2}\rangle. \tag{46}$$

To obtain $\langle(1-\coth(\alpha r))\rangle$, we choose $q=V_0$ and

$$\frac{\partial E_{n,l}}{\partial V_0} = \langle U_{n,l}(r)\left|\frac{\partial H}{\partial V_0}\right|U_{n,l}(r)\rangle = \langle(1-\coth(\alpha r))\rangle. \tag{47}$$

For $\langle(1-\coth(\alpha r))^2\rangle$, we consider $q=V_1$. Therefore

$$\frac{\partial E_{n,l}}{\partial V_1} = \langle U_{n,l}(r)\left|\frac{\partial H}{\partial V_1}\right|U_{n,l}(r)\rangle = \langle(1-\coth(\alpha r))^2\rangle. \tag{48}$$

As the final step, the expectation value $\langle T\rangle$ is obtained through the well-known relation $E_{n,l} = \langle T\rangle + \langle V(r)\rangle$. Figures 5 and 6 show that plots of $\langle(1-\coth(\alpha r))\rangle$ and $\langle(1-\coth(\alpha r))^2\rangle$ versus D for various quantum numbers respectively.

3.2. Oscillator strength

The study of transition from a quantum state to another is a source of invaluable knowledge in many areas of physics from astronomy to atomic physics.[35–37] For a transition from a lower state ψ_i to an upper state ψ_f, the equivalent length form for the absorption oscillator strength is

$$f_{ij}^{l} = \frac{2}{3}\frac{m}{\hbar^2}(E_j - E_i)|\langle\psi_j|r|\psi_i\rangle|^2. \tag{49}$$

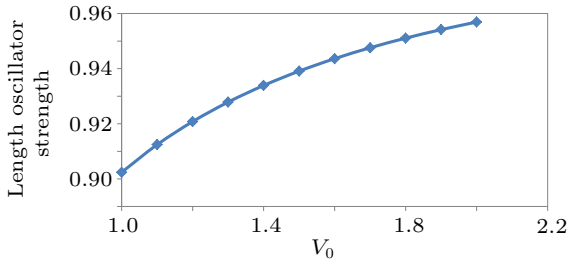


Fig. 7. (color online) Variation of the length of oscillator strength with coefficient V_0.

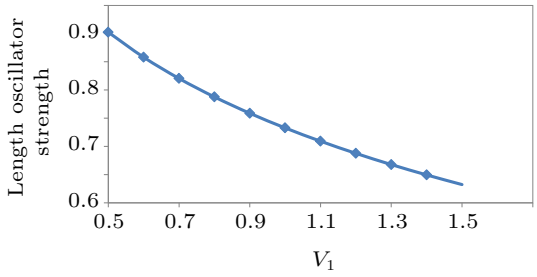


Fig. 8. (color online) Variation of the length of oscillator strength with coefficient V_1.

Figure 7 illustrates the variation of the oscillator strength with coefficient V_0 for $V_1 = 0.5$. Figure 8 shows the variation of the oscillator strength with coefficient V_1 for $V_0 = 1$. To be

sure about our results, we numerically calculate the eigenvalues as well and our results are given in Tables 1 and 2 for $\alpha = 0.05$ and $\alpha = 0.005$, respectively. The numerical results obtained by a "shooting method" based on a discrete variable representation (DVR)[38] of the Hamiltonian are in acceptable agreement with the approximate analytical ones.

Table 1. Eigenvalues for $D = 3$ for $V_0 = 1$, $V_1 = 1/2$, and $\alpha = 0.05$.

l	n	$E_{n,l}$	$E_{n,l}$ Eq. (14)
1	0	−0.421435	−0.420660
1	1	−0.302493	−0.301743
1	2	−0.208362	−0.207643
1	3	−0.135335	−0.134656
1	4	−0.080444	−0.079817
2	0	−0.408368	−0.406049
2	1	−0.292086	−0.289841
2	2	−0.200207	−0.198057
2	3	−0.129106	−0.127080

Table 2. Eigenvalues for $D = 3$ for $V_0 = 1$, $V_1 = 1/2$, and $\alpha = 0.005$.

l	n	$E_{n,l}$	$E_{n,l}$ Eq. (14)
1	0	−0.492457	−0.492449
1	1	−0.477781	−0.477773
1	2	−0.463420	−0.463413
1	3	-0.449370	-0.449363
1	4	−0.435626	−0.435618
2	0	−0.492309	−0.492285
2	1	−0.477635	−0.477612
2	2	−0.463278	−0.463255
2	3	−0.449232	−0.449208

4. Conclusion

We already know that the Coulomb potential has its own disadvantages, owing to its structure. This leads to the appearance of alternative exponential-type potentials such as the Hulthén potential, etc. In our work, we introduce the potential $V_0(1-\coth(\alpha r))+V_1(1-\coth(\alpha r))^2$ which resembles the Kratzer potential in small values of r and tends to zero for large values. To have a more general solution, we consider the Schrödinger equation in arbitrary space. As the analytical techniques provide a deeper insight into the problem, we follow the SUSYQM after replacing the centrifugal term by an appropriate exponential approximation and thereby calculate both eigenfunctions and energy eigenvalues. Instead of focusing on a particular system, we try to give rather general results and calculate some useful expectation values and oscillator strengths. The exact numerical calculation reveal that for a fixed n and various values of l and s, the energies diverge as D increases. In addition, for a fixed n, $E_{n,l}^{(D)} = E_{n,l-1}^{(D+2)}$. In all cases, for $l = 0$, $D = 0$ and $D = 2$ represent a symmetric behavior.

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