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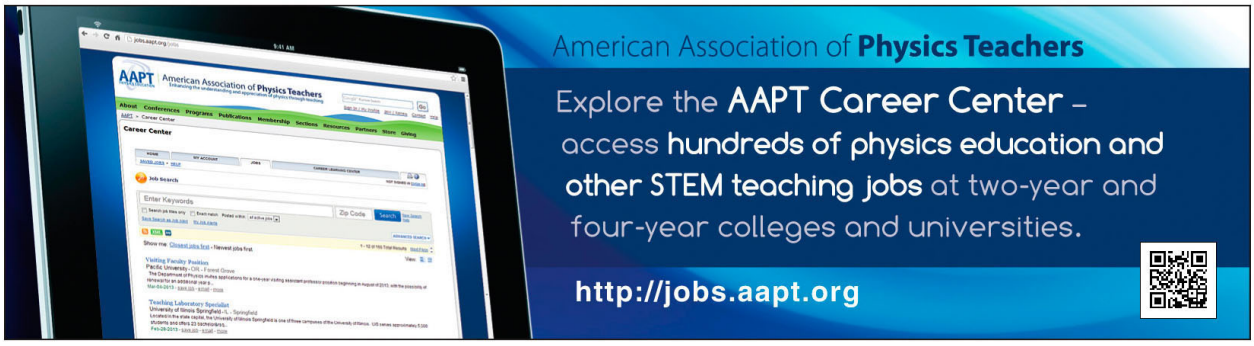

accuracy of the numerical integration; (a) requires no programming and, since it runs in FORTRAN, is substantially faster. We consider Plod in the manuscript.
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An operator solution for the Hulthén potential

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Shift operators are derived for s states of the Hulthén potential. These operators are used to obtain energy eigenvalues and normalized coordinate-space wave functions for bound s states. The condition for the existence of these states is deduced from the Hellmann–Feynman theorem, and this theorem together with the hypervirial theorem are used to calculate certain expectation values.

I. INTRODUCTION

The operator method of solving quantum mechanical problems is based on shift operators and results such as the virial, hypervirial, and Hellmann–Feynman theorems. This method has been applied to many of the quantum mechanical systems that can be solved exactly, such as the one-dimensional oscillator,[1] the theory of angular momentum,[2] and other problems.[3,4]

In the case of spherically symmetric problems in an angular momentum basis, the operator method has been used for the free particle, the isotropic three-dimensional harmonic oscillator, the Coulomb problem,[3,5] and certain generalized potentials.[6] If one considers just the s states of spherically symmetric potentials, the centrifugal term in the Hamiltonian is zero and, consequently, there are several more problems, such as the Morse and Rosen–Morse potentials,[7] that can be treated by operator methods.

The purpose of this paper is to present an operator solution for the s states of the Hulthén potential

$$V(r) = -V_0\{1/[\exp(r/a)-1]\}. \tag{1}$$

Here, V_0 and a are positive constants and $r=(\mathbf{r}\cdot\mathbf{r})^{1/2}$. This short-range potential provides a useful approximation to the internucleon potential.[8] The Schrödinger wave equation can be solved analytically for s states of the Hulthén potential and a wave-mechanical treatment for bound states is given in the text by Flügge.[9] To my knowledge, the only operator analysis for this potential is that by Green who used a factorization method to determine the energy of the ground state.[3]

A brief summary of Green's calculations is given in Sec. II. In Sec. III shift operators are derived for s states of the Hulthén potential and these are used in Sec. IV to obtain energy eigenvalues for bound s states. The condition for the existence of these states is deduced in a simple manner with the aid of the Hellmann–Feynman theorem. In Sec. V the hypervirial theorem and the Hellmann-Feynman theorem are used to calculate the coefficients in the shift operations. Normalized coordinate-space wave functions are deduced in Sec. VI.

The operator calculations presented here provide an instructive alternative to the more traditional wave-mechanical treatment. The operator method also has the merit of simplicity. For example, the normalization calculations in Sec. VI are almost trivial whereas normalization by integration is less so (see Sec. VI) and, in fact, is not given in the wave-mechanical solution of Ref. 9.

II. THE GROUND STATE

For s states of a particle of mass M in the Hulthén potential (1) the Hamiltonian is

$$H=(1/2M)p_r^2 - V_0\{1/[\exp(r/a)-1]\}. \tag{2}$$

Here,

$$p_r = \tfrac{1}{2}(\hat{\mathbf{r}}\cdot\mathbf{p}+\mathbf{p}\cdot\hat{\mathbf{r}}) = r^{-1}(\mathbf{r}\cdot\mathbf{p}-i\hbar) \tag{3}$$

is the usual radial momentum operator: It satisfies the commutation relation

$$[p_r, f(r)] = -i\hbar\frac{df}{dr}. \tag{4}$$

The energy eigenvalue equation is

$$H|E\rangle = E|E\rangle. \tag{5}$$

It is convenient to define the dimensionless quantities

$$\nu = (2Ma^2\hbar^{-2}V_0)^{1/2} \tag{6}$$

and

$$\lambda = (-2Ma^2\hbar^{-2}E)^{1/2}. \tag{7}$$

For bound states ($E<0$), λ is real.

Green[10] considered an operator C that annihilates the ground state

$$C|E_0\rangle = 0 \tag{8}$$

and factorizes the Hamiltonian (2)

$$C^\dagger C = 2M(H-E_0). \tag{9}$$

He showed that if p_r is Hermitian, the operator

$$C = ip_r - \hbar a^{-1}/[\exp(r/a) - 1] + \tfrac{1}{2}\hbar a^{-1}(\nu^2 - 1) \tag{10}$$

satisfies (9) provided

$$E_0 = -(\hbar^2/8Ma^2)(\nu^2 - 1)^2. \tag{11}$$

Equation (11) gives the energy of the ground state. The condition for this state to exist is $\nu^2 > 1$ (see Sec. IV). Thus (7) and (11) yield the relation

$$\nu^2 = 2\lambda + 1 \tag{12}$$

for the ground state.

In the coordinate representation

$$p_r = -i\hbar\left(\frac{d}{dr} + \frac{1}{r}\right) \tag{13}$$

and (8) is the first-order differential equation

$$\left(a\frac{d}{dr} - \frac{1}{\exp(r/a) - 1} + \lambda\right) r\psi_0(r) = 0 \tag{14}$$

for the ground-state wave function $\psi_0(r) = \langle r|E_0\rangle$. Integration of (14) yields

$$\psi_0(r) = c_0(r/a)^{-1}(1 - e^{-r/a})e^{-\lambda r/a}, \tag{15}$$

where c_0 is a constant. The normalization

$$\int_0^\infty |\psi_0|^2 r^2\, dr = 1 \tag{16}$$

requires

$$c_0 = 2a^{-3/2}[\lambda(\lambda + \tfrac{1}{2})(\lambda + 1)]^{1/2}. \tag{17}$$

III. SHIFT OPERATORS

It is convenient to use the dimensionless operators

$$u = r/a \tag{18}$$

and

$$p_u = (a/\hbar)p_r \tag{19}$$

that satisfy

$$[p_u, f(u)] = -i\frac{df}{du}. \tag{20}$$

By multiplying both sides of (5) on the left by $(1 - e^{-u})^2$ and rearranging terms we can rewrite this equation in the form

$$O_n|n\lambda\rangle = -\lambda^2|n\lambda\rangle, \tag{21}$$

where

$$O_n = (1 - e^{-u})^2 p_u^2 - (n^2 + \lambda^2)e^{-u} + n^2 e^{-2u}, \tag{22}$$

$$n = (\nu^2 + \lambda^2)^{1/2}, \tag{23}$$

and $|n\lambda\rangle$ denotes $|E\rangle$.

We obtain shift operators by factorizing O_n. Inspection of (22) suggests that O_n can be factorized by the operators

$$A_n^{\pm} = \pm i(1 - e^{-u})p_u + ne^{-u} + K_n^{\pm}, \tag{24}$$

where $K_n^{\pm}$ are independent of u and p_u. Using (20), (22), and (24), a short calculation shows that

$$A_{n+1}^{-}A_n^{+} = O_n + K_{n+1}^{-}K_n^{+} \tag{25}$$

and

$$A_{n-1}^{+}A_n^{-} = O_n + K_{n-1}^{+}K_n^{-}, \tag{26}$$

where

$$K_n^{+} = K_{n+1}^{-} \tag{27}$$

$$= -(n^2 + n + \lambda^2)/(2n + 1). \tag{28}$$

It follows from (25), (26), and (21) that

$$A_n^{\pm}|n\lambda\rangle = \alpha_n^{\pm}|n \pm 1, \lambda\rangle, \tag{29}$$

where the coefficients $\alpha_n^{\pm}$ are independent of u and p_u. These coefficients are calculated below (see Sec. V). According to (29) and (23) the shift operators $A_n^{\pm}$ transform between eigenkets of the same λ belonging to different potentials (different ν). (Thus the kets $|n'\lambda\rangle$ and $|n\lambda\rangle$ are not necessarily orthogonal.) Operators that transform between the eigenkets of different potential wells are also known for other potentials.[7,11]

IV. ENERGY EIGENVALUES

Equations (12) and (23) show that for the ground state

$$n = \lambda + 1. \tag{30}$$

By applying $A_{\lambda+1}^{+}, A_{\lambda+2}^{+}, \ldots$ to the ground state $|\lambda + 1, \lambda\rangle$ one obtains kets $|\lambda + 2, \lambda\rangle, |\lambda + 3, \lambda\rangle, \ldots$. In Sec. V it is shown that these kets are normalizable if the ground state is normalizable. Thus for a given Hulthén potential (ν fixed) the values of n are

$$n = N + \lambda + 1, \tag{31}$$

where

$$N = 0, 1, 2, \ldots. \tag{32}$$

[There is an upper limit to the value of N for which the potential will bind the particle—see (37).] Equations (31), (23), and (7) yield the energy eigenvalues for bound s states

$$E_N = -\frac{\hbar^2}{2Ma^2}\left(\frac{\nu^2 - (N+1)^2}{2(N+1)}\right)^2. \tag{33}$$

For the existence of these bound states there is a condition on the parameter ν. This condition can be obtained by treating V_0 as a continuous variable and applying the Hellmann–Feynman theorem[12] to (5)

$$\left\langle \frac{\partial H}{\partial V_0} \right\rangle = \frac{\partial E_N}{\partial V_0}. \tag{34}$$

Substituting (2), (33), and (6) in (34) we find

$$\langle (e^u - 1)^{-1} \rangle = [\nu^2 - (N+1)^2]/2(N+1)^2. \tag{35}$$

For bound states the left-hand side of (35) is positive because the average value of the potential (1) is negative. Therefore,

$$\nu^2 > (N+1)^2. \tag{36}$$

Thus for a given potential the number of bound states is finite and determined by[8,9]

$$V_0 > (\hbar^2/2Ma^2)(N+1)^2. \tag{37}$$

This method of determining the condition for a potential well to bind a particle can also be used for other potentials such as the Rosen–Morse potential.

V. THE COEFFICIENTS $\alpha_n^{\pm}$

If the kets in (29) are normalized,

$$|\alpha_n^{\pm}|^2 = \langle n\lambda|(A_n^{\pm})^{\dagger}A_n^{\pm}|n\lambda\rangle. \tag{38}$$

Taking the adjoints of (24) and using (27) we have

$$(A_n^+)^\dagger = A_{n+1}^- - 2e^{-u} \tag{39}$$

and

$$(A_n^-)^\dagger = A_{n-1}^+ + 2e^{-u}. \tag{40}$$

Substituting (39) and (40) in (38) and using (25), (26), and (21) we find

$$|\alpha_n^+|^2 = (K_n^+)^2 - \lambda^2 - 2\langle e^{-u}A_n^+\rangle \tag{41}$$

and

$$|\alpha_n^-|^2 = (K_n^-)^2 - \lambda^2 + 2\langle e^{-u}A_n^-\rangle. \tag{42}$$

To evaluate the expectation values on the right-hand sides of (41) and (42) we require the expectation values of $e^{-u}(1-e^{-u})p_u$, e^{-2u}, and e^{-u}. With the aid of the hypervirial theorem these can be expressed in terms of (35) (see Appendix),

$$\langle ie^{-u}(1-e^{-u})p_u\rangle = \frac{1}{2}\langle e^{-u} - 2e^{-2u}\rangle, \tag{43}$$

$$\langle e^{-2u}\rangle = [(n^2+3\lambda^2-1)/4(n^2-1)]\langle e^{-u}\rangle, \tag{44}$$

and

$$\langle e^{-u}\rangle = [2\nu^2/(4n^2-1)]\langle (e^u-1)^{-1}\rangle. \tag{45}$$

In terms of n and λ, Eq. (35) is

$$\langle (e^u-1)^{-1}\rangle = \lambda/(n-\lambda). \tag{46}$$

Substituting Eqs. (24), (27), (28), and (43)–(46) in (41) and (42), some straightforward though tedious algebra yields

$$\alpha_n^\pm = -\frac{n-\lambda\pm 1}{2n\pm 1}\left(\frac{n}{n\pm 1}(n+\lambda)(n+\lambda\pm 1)\right)^{1/2}, \tag{47}$$

where a phase factor has been set equal to -1.

We now adopt a simpler notation by letting $|N\rangle$ denote $|n\lambda\rangle$. Then (29) becomes

$$A_N^\pm |N\rangle = \alpha_N^\pm |N\pm 1\rangle, \tag{48}$$

where

$$A_N^\pm = \pm i(1-e^{-u})p_u + (N+\lambda+1)e^{-u} + K_N^\pm, \tag{49}$$

and $\alpha_N^\pm$ and $K_N^\pm$ are given by (47) and (28) with n replaced by (31). Because $|\alpha_N^+|^2 > 0$ for $N > 0$ the eigenkets $|N\rangle$ $(N = 1, 2, \ldots)$ are normalizable [provided, of course, that (37) is satisfied] if the ground state $|0\rangle$ is normalizable. Also, $\alpha_N^- = 0$ if $N = 0$ and therefore

$$A_0^-|0\rangle = 0. \tag{50}$$

Equation (50) is the same as Eq. (8) with C given by (10).

We remark that the shift operators $A_n^\pm$ can also be derived by transforming (5) into one of the standard forms considered by Infeld and Hull.[11] (The appropriate form is type E of Ref. 11.) This approach is lengthier than the *ab initio* calculations performed above. Also, it turns out that to calculate the coefficients $\alpha_n^\pm$ by using Infeld–Hull factorization, one has to evaluate $\langle V^2\rangle$ rather than $\langle V\rangle$ as in the above calculations. It is not clear how $\langle V^2\rangle$ can be calculated by operator methods.

VI. COORDINATE-SPACE WAVE FUNCTIONS

In the coordinate representation the raising operation in (48) becomes

$$\left[(1-e^{-u})\left(\frac{d}{du}+\frac{1}{u}\right) + (N+\lambda+1)e^{-u} + K_N^+\right]\psi_n(u) = \alpha_N^+\psi_{N+1}(u), \tag{51}$$

where

$$\psi_N(u) = \langle u|N\rangle \tag{52}$$

is the coordinate-space wave function. Starting with the ground state (15) it is straightforward to use (51) to calculate the wave functions of the excited states. In (51) we let

$$\psi_N(u) = c_0 u^{-1}(1-e^{-u})e^{-\lambda u}\phi_N(u), \tag{53}$$

and we substitute the expressions for K_N^+ and α_N^+. This yields the recurrence relation

$$\phi_{N+1}(u) = \beta_N D_N \phi_N(u) \quad (N = 0,1,2,\ldots), \tag{54}$$

where

$$\beta_N = \left(\frac{(N+\lambda+2)(N+2\lambda+1)(N+2\lambda+2)}{(N+\lambda+1)(N+2)^2}\right)^{1/2}, \tag{55}$$

$$D_N = 1 - \frac{2N+2\lambda+3}{N+2\lambda+1}x + \frac{2N+2\lambda+3}{(N+2\lambda+1)(N+2\lambda+2)}x(1-x)\frac{d}{dx}, \tag{56}$$

and $x = e^{-u}$. From (15) and (53), $\phi_0 = 1$. Thus by repeated application of (54) we have

$$\phi_N(u) = \beta_{N-1}\cdots\beta_1\beta_0 P_N(x) \quad (N = 1,2,\ldots), \tag{57}$$

where

$$P_N(x) = D_{N-1}\cdots D_1 D_0 1. \tag{58}$$

We evaluate (57) in two parts. Consider first $P_N(x)$. In general, $P_N(x)$ is a polynomial of order N, and the first few of these are given in Table I where we have defined $P_0 = \phi_0 = 1$.

In terms of the hypergeometric function

$${}_2F_1(a,b;c;x) = 1 + \frac{ab}{c}\frac{x}{1!} + \frac{a(a+1)b(b+1)}{c(c+1)}\frac{x^2}{2!} + \cdots, \tag{59}$$

the entries in Table I are given by

$$P_N(x) = {}_2F_1(-N, N+2\lambda+2; 2\lambda+1; x). \tag{60}$$

Using induction and (58) and (56) one can readily extend (60) to all N.

Consider next the product of the β's in (57). With β_N given by (55) this product is elementary and a short calcu-

Table I. The polynomials P_N for $N = 0$, 1, 2. For $N = 1$ and 2 the expressions for P_N are calculated from (58) and (56).

N	$P_N(x)$
0	1
1	$1 - \frac{2\lambda+3}{2\lambda+1}x$
2	$1 - \frac{2(2\lambda+4)}{2\lambda+1}x + \frac{2(2\lambda+4)(2\lambda+5)}{(2\lambda+1)(2\lambda+2)}\frac{x^2}{2}$

lation yields

$$\beta_{N-1}\cdots\beta_1\beta_0 = \frac{\Gamma(N+2\lambda+1)}{(N+1)!\Gamma(2\lambda+1)} \times\left(\frac{(N+\lambda+1)(N+2\lambda+1)}{(\lambda+1)(2\lambda+1)}\right)^{1/2}. \tag{61}$$

In writing down (61) we have used the result

$$(\alpha+n)\cdots(\alpha+1)\alpha = \Gamma(\alpha+n+1)/\Gamma(\alpha). \tag{62}$$

Substituting (57), (60), (61), and (17) in (53) we obtain the normalized Hulthén wave functions for bound s states,

$$\psi_N(u) = a^{-3/2}\frac{\Gamma(N+2\lambda+1)}{(N+1)!\Gamma(2\lambda+1)}[2\lambda(N+\lambda+1) \times(N+2\lambda+1]^{1/2}u^{-1}(1-e^{-u})e^{-\lambda u} \times{}_2F_1(-N,N+2\lambda+2;2\lambda+1;e^{-u}). \tag{63}$$

We remark that to normalize these wave functions by integration is not trivial. It can be done by expressing the hypergeometric function in terms of Jacobi polynomials, then changing variables and using tabulated integrals. These calculations are similar to those for the Rosen–Morse potential, which are given in Ref. 13.

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I would like to thank a referee for pointing out Ref. 4.

APPENDIX

We use the method given in Ref. 14 to prove Eqs. (43)–(45). According to the hypervirial theorem[14]

$$\langle[W,H]\rangle = 0. \tag{A1}$$

Here the expectation value is with respect to the eigenkets $|E\rangle$ of H, and it is assumed that H is Hermitian with respect to $W|E\rangle$; otherwise, the operator W is arbitrary.

With $W=g(r)$ and $dg/dr=f$, Eqs. (A1), (2), and (4) give

$$\langle fp_r\rangle = \frac{1}{2}i\hbar\left\langle\frac{df}{dr}\right\rangle. \tag{A2}$$

Similarly, with

$$W = f(r)p_r + \frac{1}{2}i\hbar\frac{df}{dr}$$

we obtain

$$\left\langle\frac{\hbar^2}{4M}\frac{d^3f}{dr^3} + 2(E-V)\frac{df}{dr} - \frac{dV}{dr}f\right\rangle = 0. \tag{A3}$$

Using the dimensionless operators (18) and (19), and choosing

$$f = e^{-u}(1-e^{-u}),$$

(A2) yields (43). Similarly, from (A3), (1), and (7) with

$$f = (1-e^{-u})^2$$

and

$$f = 1-e^{-u},$$

respectively, we obtain (44) and (45).

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