SOLUTION OF SCHRÖDINGER EQUATION BY LAPLACE TRANSFORM

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1. Introduction

Laplace transform techniques for solving differential equations do not seem to have been directly applied to the Schrödinger equation in quantum mechanics. This may be because the Laplace transform of a wave function, in contrast to the Fourier transform, has no direct physical significance. However, this paper will show that scattering phase shifts and bound state energies can be determined from the singularities of the Laplace transform of the wave function. The Laplace transform method can thereby simplify calculations if the potential allows a straightforward solution of the transformed Schrödinger equation. Suitable cases are the Coulomb, oscillator and exponential potentials and the Yamaguchi separable non-local potential.

In section 2, the required properties of the Laplace transform (hereafter called the transform) are stated. Then the method is used to find the energies of bound S-states in a Coulomb potential. Next the bound state energy and scattering phase shift of the Yamaguchi potential are calculated. The behaviour of the Jost function at the origin can also be found, and the exponential potential is treated in this way. Section 6 completes the solution of the Coulomb problem, and treats the three-dimensional harmonic oscillator. Finally the scalar product of two wave functions is calculated by constructing a differential operator from one transform, and applying it to the other transform. The complex conjugate of any operator defined on the transforms may then be determined directly.

The essential features of this method of finding the asymptotic form of the solution of a linear differential equation have been given in previous treatments [3, 8] of the Laguerre equation, especially that by Murnaghan, who noted the application to the hydrogen atom. The examples below show that all physically significant quantities can be obtained directly from the transforms without inverting.

An appendix records the Laplace transform of $J_\nu(\beta e^{-\frac{1}{2}r})$, obtained first by comparing Section 5 with the standard treatment of the exponential potential, and then directly in a simpler form. This is believed to be a new result.

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2. Properties of the transform

The transform of $f(r)$ is

$$F(s) = Lf(r) = \int_0^\infty e^{-sr} f(r)\, dr$$

and has the properties

(2.1) $$Lf''(r) = s^2 F(s) - f'(0) - sf(0)$$

(2.2) $$L\{e^{-br} f(r)\} = F(s+b)$$

(2.3) $$L\{r^n f(r)\} = (-1)^n F^{(n)}(s)$$

(2.4) $$F(s) \to 0 \quad \text{as} \quad s \to \infty$$

The relation between the asymptotic behaviour of $f(r)$ and the singularities of $F(s)$ is very important for the applications below. Suppose $F(s)$ is singular at $s = s_0, s_1, s_2, \cdots$, with $\mathrm{Re}\, s_0 > \mathrm{Re}\, s_1 \geqq \mathrm{Re}\, s_2 \geqq \cdots$, and that (near $s = s_0$),

$$F(s) \underset{s \to s_0}{\sim} A(s-s_0)^{-\nu}$$

Then [7, p. 102]

(2.5) $$f(r) \underset{r \to \infty}{\sim} A[\Gamma(\nu)]^{-1} r^{\nu-1} \exp(s_0 r)$$

When $\nu = 1$, $F(s)$ has a simple pole at $s = s_0$, and A is the residue. When $\mathrm{Re}\, s_0 = \mathrm{Re}\, s_1 > \mathrm{Re}\, s_2$, the asymptotic form of $f(r)$ consists of the sum of two terms like (2.5), one from s_0 and one from s_1. If $\mathrm{Re}\, s_0 > \mathrm{Re}\, s_1$, the term like (2.5) coming from s_1 is the next exponential term in the asymptotic expansion of $f(r)$.

3. Coulomb potential: bound *S*-states

This example is given first, since the standard treatment is very well-known. The potential is $V(r) = -Ze^2 r^{-1}$, and the radial equation may be written

$$ru''(r) + \alpha\lambda u(r) - \tfrac{1}{4}\alpha^2 r u(r) = 0.$$

The constants are those used by Schiff [6]:

$$\alpha^2 \hbar^2 = -8\mu E, \qquad \alpha\lambda\hbar^2 = 2\mu Z e^2, \qquad \alpha > 0.$$

Using (2.3), and (2.1) with the boundary condition $u(0) = 0$, the transformed equation is

$$-2sU(s) - s^2 U'(s) + \alpha\lambda U(s) + \tfrac{1}{4}\alpha^2 U'(s) = 0.$$

This integrates at once to give

(3.1) $$U(s) = C\left(s - \frac{\alpha}{2}\right)^{\lambda-1} \left(s + \frac{\alpha}{2}\right)^{-\lambda-1}$$

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where C is an arbitrary constant of integration. If λ is not a positive integer, then $s_0 = \alpha/2$; from (2.5) $u(r)$ is not a square-integrable function, since its asymptotic form involves $e^{\frac{1}{2}\alpha r}$. On the other hand if λ is a positive integer, $s_0 = -\alpha/2$, and (2.5) shows that $u(r)$ is square-integrable.

Thus, for the eigenvalue problem, the explicit nature of $u(r)$ is not required. Once $U(s)$ is obtained, it is only necessary to inspect its singularities. $U(s)$ is not necessarily required explicitly; in this example a power series expansion of $U(s)$ about $s = \frac{1}{2}\alpha$ may be assumed, and the indicial equation gives the condition for a singularity. In this example there is an additional advantage: the second-order equation for u transforms to an integrable first-order equation for U.

The precise asymptotic form of $u(r)$ may be written down by substituting the appropriate values of A in (2.5). For general λ this gives

$$u(r) \underset{r\to\infty}{\sim} C\left[\frac{e^{\frac{1}{2}\alpha r}}{\alpha\Gamma(1-\lambda)}\left\{(\alpha r)^{-\lambda}+\cdots\right\} - \frac{e^{-\frac{1}{2}\alpha r}}{\alpha\Gamma(1+\lambda)}\left\{(-\alpha r)^{\lambda}+\cdots\right\}\right].$$

from which the first term may be expected to vanish only when $\lambda = 1, 2, 3, \cdots$. However, this expression is not actually required to deduce the eigenvalues.

4. The Yamaguchi potential

The non-local potential with

$$V(r, r') = -\hbar^2 b^3 W(4\pi m r r')^{-1}\exp(-br-br'),$$

W a dimensionless constant, only acts in S-states, in which the radial equation is ($\hbar^2\kappa^2 = -2mE$)

$$u''(r)-\kappa^2 u(r) = -2Wb^3 e^{-br}\int_0^\infty e^{-br'}u(r')\,dr'. \tag{4.1}$$

Since the integral is just $U(b)$, the transformed equation is

$$(s^2-\kappa^2)U(s) = u'(0)-2Wb^3U(b)(s+b)^{-1}$$

which incorporates the boundary condition $u(0) = 0$. The value $s = b$ shows the relation between the normalization constants $u'(0)$ and $U(b)$. Thus

$$U(s) = U(b)\left[\frac{(b^2-\kappa^2+Wb^2)(s+b)-2Wb^3}{(s+b)(s^2-\kappa^2)}\right]$$

with simple poles at $s = \kappa$, $-\kappa$ and $-b$. Thus $s_0 = \kappa > 0$, unless the residue at $s = \kappa$ vanishes, which is the condition for a bound state:

$$(b^2-\kappa^2+Wb^2)(b+\kappa) = 2Wb^3. \tag{4.2}$$

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If $W > 1$, the potential supports a bound state with energy corresponding to $\kappa = b(W^{\frac{1}{2}}-1)$. A curious feature of this potential is that when $W > 4$, $\kappa > b$, and the asymptotic form of $u(r)$ is dominated not by the usual $e^{-\kappa r}$ term, but by an e^{-br} term.

The determination of $U(s)$ is just the usual momentum-space wave function treatment [9], with $-si$ replacing p. It seems more natural to consider the integral in (4.1) as a Laplace transform.

For the scattering problem κ^2 is replaced by $-k^2$, and the poles of $U(s)$ occur at $s_0 = ik = -s_1$, $s_2 = -b$, with $\mathrm{Re}\, s_0 = \mathrm{Re}\, s_1$. If A_{ik} and A_{-ik} are the residues at s_0 and s_1, (2.5) shows that

$$u(r) \underset{r\to\infty}{\sim} A_{-ik}e^{-ikr}+A_{ik}e^{ikr} \tag{4.3}$$

and so the phase shift δ is given by

$$e^{2i\delta} = -\frac{A_{ik}}{A_{-ik}} = \frac{(b^2+k^2+Wb^2)(b^2+k^2)-2Wb^3(b-ik)}{(b^2+k^2+Wb^2)(b^2+k^2)-2Wb^3(b+ik)}. \tag{4.4}$$

Alternatively, the Jost function can be constructed. Any solution has the transform

$$F(s) = \frac{f'(0)+sf(0)}{s^2+k^2} - \frac{2Wb^3F(b)}{(b+s)(s^2+k^2)}.$$

The value $s = b$ gives one relation between $f(0)$, $f'(0)$, and $F(b)$. From (4.3), the Jost function satisfies $A_{-ik} = 1$, $A_{ik} = 0$ giving two more equations, so that $f(0)$ is determined.

$$f(0) = 1+\frac{2W(ik-b)b^3}{(b^2+k^2)(b^2+k^2+Wb^2)}.$$

Then $0 = f(0)|_{k=-i\kappa}$ gives (4.2), and $\delta = \arg f(0)$ is equivalent to (4.4). In the usual notation $f(r)$ is $f(k, r)$, $f(0)$ is $f(k, 0)$ or $f(k)$.

5. The exponential potential

If $V(r) = -V_0 \exp(-r/a)$, the S-wave radial equation can be written

$$f''(x)+b^2e^{-x}f(x)+c^2f(x) = 0 \tag{5.1}$$

with $ax = r$, $\hbar^2b^2 = 2mV_0a^2$, $\hbar^2c^2 = 2mEa^2$. Using (2.1) and (2.2), the transform $F(s)$ satisfies the first-order difference equation

$$b^2F(s+1)+(s^2+c^2)F(s) = f'(0)+sf(0). \tag{5.2}$$

The standard method of solution [5, p. 104] is to substitute $F(s) = Z(s)V(s)$ where $Z(s)$ satisfies

$$b^2Z(s+1)+(s^2+c^2)Z(s) = 0$$

giving

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$$\varDelta V(s) = -\frac{f'(0)+sf(0)}{(s^2+c^2)Z(s)}$$

from which ($\varepsilon = 1+\varDelta$)

$$V(s) = (1-\varepsilon)^{-1}\frac{f'(0)+sf(0)}{(s^2+c^2)Z(s)} + Y_1(s) = \sum_{r=0}^{\infty}\frac{f'(0)+(s+r)f(0)}{[(s+r)^2+c^2]Z(s+r)} + Y_1(s),$$

where $Y_1(s)$ is an arbitrary function of period 1.

Since $Z(s) = (-1)^s b^{-2s}\Gamma(s+ic)\Gamma(s-ic)Y_2(s)$, where $Y_2(s)$ is another arbitrary function of period 1, the general solution of (5.2) is

$$F(s) = \Gamma(s+ic)\Gamma(s-ic) \cdot \left[(-1)^s b^{-2s} Y_1(s)Y_2(s) + \sum_{r=0}^{\infty}\frac{\{f'(0)+(s+r)f(0)\}(-1)^r b^{2r}}{\Gamma(s+r+1+ic)\Gamma(s+r+1-ic)}\right].$$

In view of (2.4), the arbitrary function $Y_1(s)Y_2(s)$ must be chosen to be identically zero. The required solution is therefore

$$F(s) = \sum_{r=0}^{\infty}\frac{\{f'(0)+(s+r)f(0)\}(-1)^r b^{2r}}{(s+ic)\cdots(s+r+ic)(s-ic)\cdots(s+r-ic)} \tag{5.3}$$

with simple poles at $-n\pm ic$ ($n = 0, 1, 2, \cdots$). The asymptotic behaviour of $f(x)$ is determined by the residues

$$A_{ic} = (2ic)^{-1}[\{f'(0)+icf(0)\}G-b^2f(0)G']$$
$$A_{-ic} = (-2ic)^{-1}[\{f'(0)-icf(0)\}\bar{G}-b^2f(0)\bar{G}']$$

with $G = {}_0F_1(1+2ic; -b^2)$.

In particular, $A_{ic} = 0$, $A_{-ic} = 1$ gives the Jost function. Solving for $f(0)$ under these conditions gives

$$[2G\bar{G}-ib^2c^{-1}(G\bar{G}'-G'\bar{G})]f(0) = 2G.$$

Since the square bracket is real, the phase shift is given by

$$\delta = \arg G = \arg {}_0F_1(1+2ic; -b^2)$$

The condition for a bound state may be obtained by putting $c = -i\kappa a$ in $f(0) = 0$. Thus κ must satisfy ${}_0F_1(1+2\kappa a; -b^2) = 0$ i.e. $J_{2\kappa a}(2b) = 0$.

If this condition is found directly by taking $c^2 = -\kappa^2 a^2$ and $f(0) = 0$ in (5.2), then the transform $U(s)$ of the radial wave function is given by (5.3) with $f(0) = 0$, $c = -i\kappa a$, and $f'(0) = u'(0)$. Thus there are simple poles at the positive values $s = \kappa a, \kappa a-1, \cdots, \kappa a-[\kappa a]$, and their residues must all vanish to get a bound state. However, it turns out that all the residues have $J_{2\kappa a}(2b)$ as a factor, so that just one condition is sufficient.

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6. The Coulomb potential

The bound S-states were deduced in Section 3. With the same notation, the radial equation for angular momentum l

$$r^2u''+\alpha\lambda ru-\tfrac{1}{4}\alpha^2r^2u-l(l+1)u = 0.$$

The transformed equation is

$$(s^2-\tfrac{1}{4}\alpha^2)U''(s)+(4s-\alpha\lambda)U'(s)-(l+2)(l-1)U(s) = 0.$$

Differentiate $(l-1)$ times, and put $V(s) = U^{(l)}(s)$. There results a first order equation for $V(s)$, giving

$$V = C(s-\tfrac{1}{2}\alpha)^{\lambda-l-1}(s+\tfrac{1}{2}\alpha)^{-\lambda-l-1}.$$

From (2.3), this is the transform of $(-r)^l u(r)$. The existence of bound states, which depends on the elimination of positive exponential terms from the asymptotic form of $u(r)$, can therefore be investigated from the singularities of $V(s)$. The required condition is that $\lambda-l$ is a positive integer, so that V has no singularity at $s = \frac{1}{2}\alpha$.

It is also convenient to treat S-states separately in the scattering problem. When $l = 0$ the radial equation is $ru''-2nku+k^2ru = 0$, with $\hbar^2k^2 = 2\mu E$, $\hbar^2nk = -\mu Ze^2$. The transformed equation integrates to

$$U = C(s+ik)^{-1-in}(s-ik)^{-1+in}.$$

Using (2.5),

$$u(r) \underset{r\to\infty}{\sim} \frac{C}{2ik}\left[\frac{(2ikr)^{-in}e^{ikr}}{\Gamma(1-in)} - \frac{(-2ikr)^{in}e^{-ikr}}{\Gamma(1+in)}\right]$$
$$= \frac{C\exp(\frac{1}{2}n\pi)}{k|\Gamma(1+in)|}\sin(kr-n\log 2kr+\eta_0)$$

with $\eta_0 = \arg\Gamma(1+in)$.

When $l > 0$, the radial equation is transformed, and then differentiated $(l-1)$ times, as in the bound state case.

Integrating gives

$$U^{(l)}(s) = C(s+ik)^{-in-l-1}(s-ik)^{in-l-1}.$$

Using (2.3) and (2.5),

$$(-r)^l u(r) \underset{r\to\infty}{\sim} \frac{Ce^{\frac{1}{2}n\pi}r^l}{(2k)^{l+1}}\left[\frac{(2kr)^{-in}e^{ikr}}{i^{l+1}\Gamma(l+1-in)} + \frac{(2kr)^{in}i^{l+1}e^{-ikr}}{\Gamma(l+1+in)}\right].$$

The usual manipulation into sine form gives the phase shift.

Differentiating $(l-1)$ times can be avoided by transforming the equation for $w(r) = r^l u(r)$. This is the best method for the three-dimensional

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harmonic oscillator. Taking $(2m)^{-1}K^2\hbar^2r^2$ as the potential for a particle of mass m, and putting $mE = 2\hbar^2K\gamma$ $(K > 0)$, the radial equation is

$$u''(r)+\{4K\gamma-r^2K^2-l(l+1)r^{-2}\}u(r) = 0.$$

Then

$$r^2w''-2lrw'+4K\gamma r^2w-K^2r^4w = 0.$$

Changing the variable to $r^2 = x$, and then transforming, gives an integrable first order equation for $W(t)$, the transform of $w(x)$. When $l = 0$, $w'(x) \to \infty$ as $x \to 0$, so xw'' should not be transformed by successive use of (2.1) and (2.3), but by using

$$L(xw'') = -\lim_{x\to 0} (xw')-Lw'+tL(xw').$$

(This is also required in section 3.) The solution is

$$W = C(t-\tfrac{1}{2}K)^{\gamma-\frac{1}{2}l-\frac{3}{4}}(t+\tfrac{1}{2}K)^{-\gamma-\frac{1}{2}l-\frac{3}{4}}.$$

The eigenvalues are determined by the condition that $\gamma-\frac{1}{2}l-\frac{3}{4}$ must be a non-negative integer N, so that

$$mE = \hbar^2K(l+2N+\tfrac{3}{2}),\quad N = 0, 1, 2, 3, \cdots.$$

The Laplace transform method can also be used when the Coulomb problem is solved in the parabolic coordinates $\xi = r+z$, $\eta = r-z$, ϕ. Assuming a bound state wave function $f(\xi)g(\eta)e^{im\phi}$, and separating variables, gives [6]

$$\xi^2(4f''-\tfrac{1}{4}\alpha^2f)+\xi(4f'+\beta f)-m^2f = 0$$

where β is a separation constant. $g(\eta)$ satisfies the same equation with β replaced by $2\alpha\lambda-\beta$. Substituting $f = \xi^{1-\frac{1}{2}|m|}w$ gives

$$\xi^2(4w''-\tfrac{1}{4}\alpha^2w)+\xi\{4(3-|m|)w'+\beta w\}+4(1-|m|)w = 0.$$

The transformed equation is $(m \neq 0)$

$$(4x^2-\tfrac{1}{4}\alpha^2)W''(x)+(4x+4|m|x-\beta)W'(x) = 0.$$

Integrating,

$$W'(x) = A(x-\tfrac{1}{4}\alpha)^{(\beta/2\alpha)-\frac{1}{2}|m|-\frac{1}{2}}(x+\tfrac{1}{4}\alpha)^{-(\beta/2\alpha)-\frac{1}{2}|m|-\frac{1}{2}} \tag{6.1}$$

Similarly, substituting $g = \eta^{1-\frac{1}{2}|m|}v$, gives

$$V'(y) = B(y-\tfrac{1}{4}\alpha)^{-(\beta/2\alpha)+\lambda-\frac{1}{2}|m|-\frac{1}{2}}(y+\tfrac{1}{4}\alpha)^{(\beta/2\alpha)-\lambda-\frac{1}{2}|m|-\frac{1}{2}} \tag{6.2}$$

where $V(y)$ is the transform of $v(\eta)$.

A bound state requires that (6.1) is regular at $x = \frac{1}{4}\alpha$, and (6.2) regular at $y = \frac{1}{4}\alpha$. Thus

$\beta/\alpha = |m|+1+2n_1$ $(n_1 = 0, 1, 2, \cdots)$, and $\lambda = n_1+n_2+|m|+1$ $(n_2 = 0, 1, 2, \cdots)$.

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When $m = 0$, the equation for f can be transformed directly after dividing by ξ. The same procedure leads to $\lambda = n_1+n_2+1$ $(n_1, n_2 = 0, 1, 2, \cdots)$.

7. Evaluation of scalar products

In some of the above examples, the transform is simpler than the wave function. To exploit this fully requires some way of obtaining expectation values directly from the transform. The operators $-d/ds$ and s acting on the transform correspond to the operators r and d/dr acting on $u(r)$. The only problem is to find what operation on the transforms $U(s)$, $V(s)$ corresponds to taking the scalar product $\int_0^\infty \bar{u}(r)v(r)dr$. This is also needed to discuss normalization of transforms.

For example, the bound Coulomb S-states have normalized radial wave functions [6]

$$u_n(r) = 2^{-\frac{1}{2}}\alpha^{\frac{3}{2}}(r+\cdots)\exp(-\tfrac{1}{2}\alpha r)$$

where $(r+\cdots)$ is a polynomial in r. Taking the transform gives

$$U_n(s) = 2^{-\frac{1}{2}}\alpha^{\frac{3}{2}}\left(-\frac{d}{ds}+\cdots\right)(s+\tfrac{1}{2}\alpha)^{-1} = 2^{-\frac{1}{2}}\alpha^{\frac{3}{2}}[(s+\tfrac{1}{2}\alpha)^{-2}+\cdots]$$

which is an expansion of the normalized transform in inverse powers of $(s+\frac{1}{2}\alpha)$. Writing (3.1) in this way gives $(\lambda = n)$

$$U_n(s) = C_n\sum_{m=0}^{n-1}(-\alpha)^m\binom{n-1}{m}(s+\tfrac{1}{2}\alpha)^{-m-2}. \tag{7.1}$$

The $m = 0$ term shows that the normalized transform is obtained by choosing $C_n = 2^{-\frac{1}{2}}\alpha^{\frac{3}{2}}$. This will later be deduced directly from the transform.

Now consider $v(r)$ or $V(s)$ as the representative of a ket. The bra corresponding to $u(r)$ is represented by the function with the value $\int_0^\infty \bar{u}(r)v(r)dr$ at the argument $v(r)$; the bra maps the radial functions $v(r)$ into the scalar products $\int_0^\infty \bar{u}v dr$, and must also map the transforms $V(s)$ into the same numbers.

Let $u(r) = e^{-ar}$. Then $\int_0^\infty \bar{u}(r)v(r)dr = V(\bar{a})$. Hence the bra corresponding to $U(s) = (s+a)^{-1}$ is represented by the function which maps the transform $V(s)$ into $V(\bar{a})$. In other words the scalar product of $(s+a)^{-1}$ and $V(s)$ is $V(\bar{a})$.

Similarly if $u(r) = r^n e^{-ar}$, $\int_0^\infty \bar{u}(r)v(r)dr = (-1)^n V^{(n)}(\bar{a})$. This result was given by Cremonesi [1], who applied the Schmidt orthonormalization procedure to a set of functions of the type $u(r)$, by working in terms of the transforms. From the present viewpoint the result may be recorded in the form that the scalar product of $(s+a)^{-n}$ and $V(s)$ is

$$(-1)^{n-1}[(n-1)!]^{-1}V^{(n-1)}(\bar{a}).$$

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Since any radial function $u(r)$ can be expanded in a series of terms like $r^n e^{-ar}$, with a real, any transform can be expanded in a series of terms like $(s+a)^{-n}$. Then as the operation of taking the scalar product depends anti-linearly on the bra, the above result is sufficient. When using the transforms, scalar products are obtained by differentiation instead of the usual integration. In the bound state examples above, the transforms are rational functions, which must be expressed in partial fractions to obtain the appropriate differential operators.

Thus (7.1) shows that the scalar product of $U_n(s)$ and any $V(s)$ is

$$-\bar{C}_n \sum_{m=0}^{n-1} \alpha(gk)^m[(m+1)!]^{-1}\binom{n-1}{m} V^{(m+1)}(\tfrac{1}{2}\alpha).$$

In particular, $U_1(s) = C_1(s+\frac{1}{2}\alpha)^{-2}$ has length

$$-|C_1|^2 \frac{d}{ds}(s+\tfrac{1}{2}\alpha)^{-2}|_{s=\frac{1}{2}\alpha} = 2|C_1|^2\alpha^{-3}$$

showing that $C_1 = 2^{-\frac{1}{2}}\alpha^{\frac{3}{2}}$ is required to normalize the transform.

The complex conjugate of an operator acting on the transforms may now be found directly. Consider, for example, the operator s. The scalar product of $(-1)^n n!(s+a)^{-n-1}$ and $sV(s)$ is (taking a real)

$$\frac{d^n}{ds^n}(sV)|_{s=a} = aV^{(n)}(a)+nV^{(n-1)}(a).$$

This is also the scalar product with V of

$$a(-1)^n n!(s+a)^{-n-1}+(-1)^{n-1}n!(s+a)^{-n} = (-s)(-1)^n n!(s+a)^{-n-1}.$$

The complex conjugate of s is therefore $-s$, which is expected since s is equivalent to d/dr. Similarly d/ds can be shown to be Hermitian. The scaling operator $S(b)$ defined by $V(bs) = S(b)V(s)$ is almost unitary when b is real, for

$$\frac{d^n}{ds^n}V(bs)|_{s=a} = b^n V^{(n)}(ba)$$

which is the scalar product of

$$(-1)^n n!\,b^n(s+ab)^{-n-1} = (-1)^n n!\,b^n b^{-n-1}(sb^{-1}+a)^{-n-1}$$

with $V(s)$. Hence $\bar{S}(b) = b^{-1}S(b^{-1})$, and $b^{\frac{1}{2}}S(b)$ is unitary.

These results will now be used to find the normalization constant in (3.1). Put $\lambda = n$, and $\alpha = 2Z/na$, where the Bohr radius a is independent of n. If

$$|n\rangle = \frac{(s-Z/na)^{n-1}}{(s+Z/na)^{n+1}} = \frac{n^2(ns-Z/a)^{n-1}}{(ns+Z/a)^{n+1}}$$

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then the scaling operator gives

$$S\left(\frac{n}{n-1}\right)|n-1\rangle = \frac{(n-1)^2(ns-Z/a)^{n-2}}{(ns+Z/a)^n}$$

and so

$$|n\rangle = \frac{n^2}{(n-1)^2}\frac{(ns-Z/a)}{(ns+Z/a)}S\left(\frac{n}{n-1}\right)|n-1\rangle.$$

Hence

$$\langle n|n\rangle = \frac{n^4}{(n-1)^4}\frac{(n-1)}{n}\langle n-1|S\left(\frac{n-1}{n}\right)\frac{(-ns-Z/a)(ns-Z/a)}{(-ns+Z/a)(ns+Z/a)}S\left(\frac{n}{n-1}\right)|n-1\rangle$$

so

$$n^{-3}\langle n|n\rangle = (n-1)^{-3}\langle n-1|n-1\rangle = \langle 1|1\rangle = 2(2Z/a)^{-3}$$

by putting $\alpha = 2Z/a$ in the previous determination of the length of $U_1(s)$.

Normalization factors for the transforms may also be calculated from a formula given by Kac [2]; a similar formula given by Puri and Weygandt [4] gives any scalar product. For the normalization of (3.1), Kac's formula involves two $(\lambda+1)^{\text{th}}$ order determinants, and Puri and Weygandt's formula involves two $(2\lambda+2)^{\text{th}}$ order determinants. However, using these formulas has the advantage that the transforms do not have to be expressed in partial fractions. For the scalar product of two different transforms, the method given here has the advantage of applying when only one of the transforms is a rational function.

Appendix

The usual solution of the exponential potential is based on the fact that $f(x) = J_{2\kappa a}(2be^{-\frac{1}{2}x})$ is a solution of (5.1) with $-\kappa^2a^2$ replacing c^2. The transform is obtained from (5.3) by the substitutions $c = -i\kappa a$, $f(0) = J_{2\kappa a}(2b)$, and $f'(0) = -bJ'_{2\kappa a}(2b)$. The result can be written

$$(1)\quad \begin{aligned} LJ_\nu(\beta e^{-\frac{1}{2}r}) &= \sum_{n=0}^{\infty}\frac{\{-2\beta J'_\nu(\beta)+4(s+n)J_\nu(\beta)\}(-\beta^2)^n}{\{4s^2-\nu^2\}\{4(s+1)^2-\nu^2\}\cdots\{4(s+n)^2-\nu^2\}} \\ &= 2\beta^{1-2s}\{J_\nu(\beta)s'_{2s-1,\nu}(\beta)-J'_\nu(\beta)s_{2s-1,\nu}(\beta)\} \end{aligned}$$

where $s_{\mu,\nu}$ is a Lommel function.

Alternatively, using

$$Lf(\beta e^{-\alpha r}) = \frac{1}{\alpha\beta}\int_0^\beta\left(\frac{x}{\beta}\right)^{(s/\alpha)-1}f(x)dx,$$

$$\begin{aligned} LJ_\nu(\beta e^{-\frac{1}{2}r}) &= 2\beta^{-2s}\int_0^\beta x^{2s-1}J_\nu(x)dx \\ &= \frac{\beta^\nu\,{}_1F_2(s+\frac{1}{2}\nu;\, s+\frac{1}{2}\nu+1,\, \nu+1;\, -\frac{1}{4}\beta^2)}{2^{\nu-1}(2s+\nu)\Gamma(\nu+1)}. \end{aligned}$$

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This must be equivalent to (1), and is evidently the simplest form of the result.

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