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1983 J. Phys. A: Math. Gen. 16 263

(http://iopscience.iop.org/0305-4470/16/2/009)

J. Phys. A: Math. Gen. 16 (1983) 263–270. Printed in Great Britain

A recurrence formula for obtaining certain matrix elements in the base of eigenfunctions of the Hamiltonian for a particular screened potential

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Received 19 January 1982, in final form 23 August 1982

Abstract. A recurrence formula for obtaining matrix elements of products of powers of $\exp(-\nu r)$ and $1-\exp(-\nu r)$ is derived. The matrix elements are calculated in the base of eigenfunctions of the Hamiltonian for the effective potential $-\lambda \exp(-\nu r)/[1-\exp(-\nu r)]+\mu \exp(-\nu r)/[1-\exp(-\nu r)]^2$, where λ, ν and μ are positive constants. This potential can be considered as a generalisation of a potential suggested by Hylleraas and Risberg and by Hulthén. In the limit of the parameter ν tending to zero the recurrence formula is transformed into a recurrence formula given by Badawi *et al* for matrix elements of powers of r for the hydrogen atom.

1. Introduction

The usefulness of exactly solvable models of atomic potentials has been pointed out by, for example, Lindhard and Winther (1971). In a previous paper by this author (Myhrman 1980) the radial Schrödinger equation

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}+V(r)+\frac{l(l+1)\hbar^2}{2mr^2}\right)u=Eu, \tag{1}$$

where we use standard notations, has been solved when the effective potential is

$$V_{\text{eff}}(r)=V(r)+\frac{l(l+1)\hbar^2}{2mr^2}=-\frac{\lambda}{e^{\nu r}-1}+\frac{\mu\, e^{\nu r}}{(e^{\nu r}-1)^2}=-\frac{\lambda-\mu}{e^{\nu r}-1}+\frac{\mu}{(e^{\nu r}-1)^2}. \tag{2}$$

The potential has the proper general characteristics for a diatomic molecule potential function, as pointed out by Manning and Rosen (1933). The matrix elements derived in this paper can thus be used in calculating rotation–vibration intensities in diatomic molecules. The constants involved must of course in this case be given an appropriate interpretation.

In this paper we let $V(r)$ represent an attractive screened Coulomb potential, which tends to Ze^2/r as $\nu \to 0$, and choose

$$\lambda=\nu Ze^2 \tag{3a}$$

$$\mu=\nu^2 l(l+1)\hbar^2/2m \tag{3b}$$

where Ze is the charge of the nucleon. For physical reasons we choose the constants

ν and l such that $\nu > 0$ and $l \geq 0$, which, according to (3a, b), implies that $\lambda > 0$ and $\mu \geq 0$.

A more detailed investigation of the effective potential (2) is made by Myhrman (1980). We should only point out here that, according to (3a, b), a change of the value of l implies a change of the physical potential $V(r)$.

Introducing the new constants

$$a = 2mE/\hbar^2\nu^2 \tag{4a}$$

$$b = 2m(\lambda - \mu)/\hbar^2\nu^2 \tag{4b}$$

and the new variable

$$z = \nu r, \tag{5}$$

the radial Schrödinger equation (1) with $V(r) + l(l+1)\hbar^2/2mr^2$ given by (2) can, by means of (3b), (4a, b) and (5), be written

$$\frac{d^2u}{dz^2} + \left(a + \frac{b}{e^z - 1} - \frac{l(l+1)}{(e^z - 1)^2}\right) u = 0. \tag{6}$$

For $l = 0$ this equation is simplified into equation (5.4) given by Hylleraas and Risberg (1941) and equation (6) given by Hulthén (1942).

For the bound state problem the energy $E < 0$, which according to (4a) implies that $\sqrt{-a}$ is a real parameter. This parameter shall be chosen to be positive. Imposing the boundary conditions

$$u(0) = 0 \tag{7a}$$

$$u(r) \to 0 \qquad r \to \infty \tag{7b}$$

and normalising u according to

$$\int_0^\infty |u|^2 \, dr = 1, \tag{8}$$

we get the normalised solutions of (6) as

$$u_{k-1} = \left(\nu \frac{2\sqrt{-a}(l + k + \sqrt{-a})\Gamma(2l + 1 + k)\Gamma(2l + 1 + k + 2\sqrt{-a})}{(l + k)\Gamma(k)\Gamma(k + 2\sqrt{-a})}\right)^{1/2} \frac{1}{\Gamma(2l + 2)}$$
$$\times e^{-z\sqrt{-a}}(1 - e^{-z})^{l+1} F(-(k-1), 2l + 1 + k + 2\sqrt{-a}; 2l + 2; 1 - e^{-z}) \tag{9}$$

where k is a positive integer fulfilling the inequality

$$0 < k < [b + l(l+1)]^{1/2} - l \tag{10}$$

and where the conditions

$$\text{Re}(2\sqrt{-a}) > 0 \tag{11a}$$

and

$$\text{Re}(2l + 2) > 0 \tag{11b}$$

have to be fulfilled in order to make the integral in (8) convergent. The energy eigenvalues are obtained as

$$E = -\frac{\hbar^2\nu^2}{8m}\left(\frac{b + l(l+1)}{k + l} - k - l\right)^2 \tag{12}$$

where k is a positive integer fulfilling (10). A detailed derivation of the normalised eigenfunctions and the energy eigenvalues is given by Myhrman (1980).

Specialising (9), (10) and (12) to $l=0$, we obtain formulae given by Hulthén (1942, § 1). Inserting ($3a$, b) and ($4a$, b) into (12), letting the parameter $\nu \to 0$, putting $Z=1$ and noting that $k+l=n$ is the principal quantum number, we get the energy eigenvalues for the hydrogen atom.

2. Definition and calculation of the matrix elements $\mathcal{M}^{A,B}_{k-1,k'-1}$

Assuming that

$$\operatorname{Re}(A+\sqrt{-a_k}+\sqrt{-a_{k'}})>0 \tag{13a}$$

and

$$\operatorname{Re}(B+2l+3)>0, \tag{13b}$$

A and B being integers, we define the matrix elements of products of the Ath power of $e^{-\nu r}$ and the Bth power of $1-e^{-\nu r}$ as

$$\mathcal{M}^{A,B}_{k-1,k'-1}=\langle u_{k-1}|(e^{-\nu r})^A(1-e^{-\nu r})^B|u_{k'-1}\rangle=\int_0^\infty u^*_{k-1}(e^{-\nu r})^A(1-e^{-\nu r})^B u_{k'-1}\,dr. \tag{14}$$

In order to obtain a recurrence formula for matrix elements $\mathcal{M}^{A,B}_{k-1,k'-1}$ we shall use the factorisation method (Infeld 1941, Infeld and Hull 1951). Introducing the new independent variable

$$\zeta=\ln[\tanh(z/4)] \tag{15}$$

and putting

$$u_{k-1}=[(4/a_0\nu)\sinh(z/2)]^{1/2}G_{k+l-1/2} \tag{16}$$

where

$$a_0=\hbar^2/me^2 \tag{17}$$

is the Bohr radius, we can, if we use ($4a$) and (12), write the differential equation (6) as

$$\frac{d^2G_{k+l-1/2}}{d\zeta^2}+\frac{1}{\sinh^2\xi}\left[\frac{1}{4}-\left(\frac{b+l(l+1)}{k+l}\right)^2-(k+l)^2+2[b+l(l+1)]\cosh\zeta\right]G_{k+l-1/2}$$
$$-(l+\tfrac{1}{2})^2G_{k+l-1/2}=0. \tag{18}$$

This equation can be factorised as

$$\left(-\frac{b+l(l+1)}{k+l}\,\frac{1}{\sinh\zeta}+(k+l-\tfrac{1}{2})\coth\zeta-\frac{d}{d\zeta}\right)$$
$$\times\left(-\frac{b+l(l+1)}{k+l}\,\frac{1}{\sinh\zeta}+(k+l-\tfrac{1}{2})\coth\zeta+\frac{d}{d\zeta}\right)G_{k+l-1/2}$$
$$=[(k+l-\tfrac{1}{2})^2-(l+\tfrac{1}{2})^2]G_{k+l-1/2} \tag{19a}$$

and as

$$\left(-\frac{b+l(l+1)}{k+l}\frac{1}{\sinh\zeta}+(k+l+\tfrac{1}{2})\coth\zeta+\frac{d}{d\zeta}\right)$$
$$\times\left(-\frac{b+l(l+1)}{k+l}\frac{1}{\sinh\zeta}+(k+l+\tfrac{1}{2})\coth\zeta-\frac{d}{d\zeta}\right)G_{k+l-1/2}$$
$$=[(k+l+\tfrac{1}{2})^2-(l+\tfrac{1}{2})^2]G_{k+l-1/2}. \tag{19b}$$

We now define the operators $H_t^{\pm}$ according to

$$H_t^{\pm}=\left(-\frac{b+l(l+1)}{k+l}\frac{1}{\sinh\zeta}+t\coth\zeta\mp\frac{d}{d\zeta}\right) \tag{20}$$

where k is a fixed parameter and t is a parameter which can take on different values differing from each other by an arbitrary integer. Let then $\ldots G_{t-2}, G_{t-1}, G_t, G_{t+1}, G_{t+2}\ldots$ be a sequence of real functions fulfilling the relations

$$H_t^-G_t=[(t-l-\tfrac{1}{2})(t+l+\tfrac{1}{2})]^{1/2}G_{t-1} \tag{21a}$$

and

$$H_t^+G_{t-1}=[(t-l-\tfrac{1}{2})(t+l+\tfrac{1}{2})]^{1/2}G_t \tag{21b}$$

for an arbitrary value of the index t. From (21a, b) it follows that

$$H_t^+H_t^-G_t=[t^2-(l+\tfrac{1}{2})^2]G_t \tag{22a}$$

and from (21a, b) with t replaced by $t+1$ it follows that

$$H_{t+1}^-H_{t+1}^+G_t=[(t+1)^2-(l+\tfrac{1}{2})^2]G_t. \tag{22b}$$

In order that the definition of G_t be consistent, the functions G_t have to fulfil (22a, b) for any possible value of t. Inserting the definition (20) into (22a) and the corresponding definition of $H_{t+1}^{\pm}$ into (22b), we get

$$\left(-\frac{b+l(l+1)}{k+l}\frac{1}{\sinh\zeta}+t\coth\zeta-\frac{d}{d\zeta}\right)\left(-\frac{b+l(l+1)}{k+l}\frac{1}{\sinh\zeta}+t\coth\zeta+\frac{d}{d\zeta}\right)G_t$$
$$=[t^2-(l+\tfrac{1}{2})^2]G_t \tag{23a}$$

and

$$\left(-\frac{b+l(l+1)}{k+l}\frac{1}{\sinh\zeta}+(t+1)\coth\zeta+\frac{d}{d\zeta}\right)$$
$$\times\left(-\frac{b+l(l+1)}{k+l}\frac{1}{\sinh\zeta}+(t+1)\coth\zeta-\frac{d}{d\zeta}\right)G_t$$
$$=[(t+1)^2-(l+\tfrac{1}{2})^2]G_t. \tag{23b}$$

Comparing (19a, b) and (23a, b) we realise immediately that G_t is a solution of (18) when $t=k+l-\frac{1}{2}$.

The necessary condition for G_t to be quadratically integrable is (cf p 25 in Infeld and Hull (1951))

$$t-l-\tfrac{1}{2}=v=\text{integer}\geqslant 0. \tag{24}$$

For $t = l+\frac{1}{2}$ we obtain from (20) and (21a) the differential equation

$$\left(-\frac{b+l(l+1)}{k+l}\frac{1}{\sinh\zeta}+(l+\tfrac{1}{2})\coth\zeta+\frac{\mathrm{d}}{\mathrm{d}\zeta}\right)G_{l+1/2}=0, \tag{25}$$

the general solution of which is

$$G_{l+1/2}=N[1-\exp(-4\tanh^{-1}\mathrm{e}^{\zeta})]^{l+1/2}\exp\left[-2\left(\frac{b+l(l+1)}{k+l}-l-\tfrac{1}{2}\right)\tanh^{-1}\mathrm{e}^{\zeta}\right] \tag{26}$$

where N is an arbitrary constant factor. Assuming that

$$\mathrm{Re}\left(\frac{b+l(l+1)}{k+l}-l\right)>0 \tag{27a}$$

and

$$\mathrm{Re}(2l+1)>0, \tag{27b}$$

we obtain from (26)

$$\int_{-\infty}^{0}(G_{l+1/2})^2\,\mathrm{d}\zeta=N^2\Gamma(2l+1)\frac{\Gamma\left(\dfrac{b+l(l+1)}{k+l}-l\right)}{\Gamma\left(\dfrac{b+l(l+1)}{k+l}+l+1\right)}. \tag{28}$$

Using (21a, b) we can easily show that

$$\int_{-\infty}^{0}(G_{l+1/2+v})^2\,\mathrm{d}\zeta=\int_{-\infty}^{0}(G_{l+1/2})^2\,\mathrm{d}\zeta \tag{29}$$

where v is an arbitrary positive integer. Let us choose $v=k-1$. The left-hand side of (29) can then also be expressed in the functions u. Using (5), (15) and (16), we get

$$\int_{-\infty}^{0}(G_{k+l-1/2})^2\,\mathrm{d}\zeta=\frac{a_0\nu^2}{2}\left(\int_0^\infty u_{k-1}\frac{1}{(1-\mathrm{e}^{-\nu r})^2}u_{k-1}\,\mathrm{d}r-\int_0^\infty u_{k-1}\frac{1}{1-\mathrm{e}^{-\nu r}}u_{k-1}\,\mathrm{d}r\right). \tag{30}$$

Since the function u_{k-1} is normalised according to (8), (30) can be written

$$\int_{-\infty}^{0}(G_{k+l-1/2})^2\,\mathrm{d}\zeta=\frac{a_0\nu^2}{2}\left(\left\langle\frac{1}{(1-\mathrm{e}^{-\nu r})^2}\right\rangle-\left\langle\frac{1}{1-\mathrm{e}^{-\nu r}}\right\rangle\right). \tag{31}$$

Inserting formulae (4a) and (12) and formulae (47′) and (50′) of Myhrman (1980), namely

$$\langle(1-\mathrm{e}^{-\nu r})^{-1}\rangle=(l+k+\sqrt{-a_k})/(l+k) \tag{32a}$$

$$\langle(1-\mathrm{e}^{-\nu r})^{-2}\rangle=(l+k+\sqrt{-a_k})(2l+1+2\sqrt{-a_k})/(l+k)(2l+1), \tag{32b}$$

into (31), we obtain

$$\int_{-\infty}^{0}(G_{k+l-1/2})^2\,\mathrm{d}\zeta=\frac{a_0\nu^2}{4}\frac{\left(\dfrac{b+l(l+1)}{k+l}+k+l\right)\left(\dfrac{b+l(l+1)}{k+l}-k-l\right)}{(k+l)(2l+1)}. \tag{33}$$

Equations (28), (29) and (33) then give us

$$N=(-1)^{k-1}\left(\frac{a_0\nu^2}{4}\frac{\left(\frac{b+l(l+1)}{k+l}+k+l\right)\left(\frac{b+l(l+1)}{k+l}-k-l\right)\Gamma\left(\frac{b+l(l+1)}{k+l}+l+1\right)}{(k+l)\Gamma(2l+2)\Gamma\left(\frac{b+l(l+1)}{k+l}-l\right)}\right)^{1/2}. \tag{34}$$

From (26) and (34) the function $G_{l+1/2}$ is now completely determined.

The general matrix elements of $(e^{-\nu r})^A(1-e^{-\nu r})^B$ are defined by (14). For fixed k and k' we also define

$$\mathcal{N}^{A,B}_{v,v'}=\frac{2}{a_0\nu^2}\int_{-\infty}^{0}G_{l+1/2+v}(e^{-\nu r})^{A-1}(1-e^{-\nu r})^{B+2}G_{l+1/2+v'}\,d\zeta \tag{35}$$

which for the special choice $v=k-1$ and $v'=k'-1$ gives

$$\mathcal{N}^{A,B}_{k-1,k'-1}=\mathcal{M}^{A,B}_{k-1,k'-1}. \tag{36}$$

In order to get explicit expressions for an arbitrary matrix element we have to calculate $\mathcal{N}^{A,B}_{v,v'}$ for $v=v'=0$, i.e.

$$\mathcal{N}^{A,B}_{0,0}=\frac{2}{\nu^2a_0}\int_{-\infty}^{0}G_{l+1/2}(e^{-\nu r})^{A-1}(1-e^{-\nu r})^{B+2}G_{l+1/2}\,d\zeta. \tag{37}$$

In order to make the integral in (37) convergent we assume

$$\mathrm{Re}\left[A-l-1+\frac{1}{2}\left(\frac{b+l(l+1)}{k+l}+\frac{b+l(l+1)}{k'+l}\right)\right]>0 \tag{38a}$$

and

$$\mathrm{Re}(B+2l+3)>0. \tag{38b}$$

From equation (37) with (26) and (34) inserted we then get

$$\begin{aligned}\mathcal{N}^{A,B}_{0,0}&=(-1)^{k+k'}\\&\times\left(\frac{\left(\frac{b+l(l+1)}{k+l}+k+l\right)\left(\frac{b+l(l+1)}{k+l}-k-l\right)\left(\frac{b+l(l+1)}{k'+1}+k'+l\right)\left(\frac{b+l(l+1)}{k'+1}-k'-l\right)}{(k+l)(k'+l)}\right.\\&\quad\left.\times\frac{\Gamma\left(\frac{b+l(l+1)}{k+l}+l+1\right)\Gamma\left(\frac{b+l(l+1)}{k'+l}+l+1\right)}{\Gamma\left(\frac{b+l(l+1)}{k+l}-l\right)\Gamma\left(\frac{b+l(l+1)}{k'+l}-l\right)}\right)^{1/2}\\&\quad\times\frac{\Gamma(2l+3+B)\Gamma\left(\frac{[b+l(l+1)](k+k'+2l)}{2(k+l)(k'+l)}-l-1+A\right)}{2\Gamma(2l+2)\Gamma\left(\frac{[b+l(l+1)](k+k'+2l)}{2(k+l)(k'+l)}+l+2+A+B\right)}.\end{aligned} \tag{39}$$

If we now choose $k = k' = 1$ in (39) we get the matrix element

$$\mathcal{M}_{0,0}^{A,B} = \frac{\Gamma(2l+3+B)\Gamma\left(\frac{b+l(l+1)}{l+1}+l+2\right)\Gamma\left(\frac{b+l(l+1)}{l+1}-l-1+A\right)}{\Gamma(2l+3)\Gamma\left(\frac{b+l(l+1)}{l+1}-l-1\right)\Gamma\left(\frac{b+l(l+1)}{l+1}+l+2+A+B\right)} \tag{40}$$

or in another notation

$$\mathcal{M}_{0,0}^{A,B} = \frac{\Gamma(2l+3+B)\Gamma(2l+3+2\sqrt{-a_1})\Gamma(A+2\sqrt{-a_1})}{\Gamma(2l+3)\Gamma(2\sqrt{-a_1})\Gamma(2l+3+A+B+2\sqrt{-a_1})} \tag{41}$$

where $\sqrt{-a_1}$ is defined by ($4a$) and (12) with $k=1$ inserted.

Returning to formula (35) we find by means of ($21a, b$) that for $v > 0$

$$\begin{aligned}\mathcal{N}_{v,v'}^{A,B} &= \frac{2}{a_0 \nu^2}[v(2l+v+1)]^{-1/2}\int_{-\infty}^{0}(H_{l+1/2+v}^{+}G_{l-1/2+v})\\ &\quad\times(e^{-\nu r})^{A-1}(1-e^{-\nu r})^{B+2}G_{l+1/2+v'}\,d\zeta\\ &= \frac{2}{a_0\nu^2}[v(2l+v+1)]^{-1/2}\int_{-\infty}^{0}G_{l-1/2+v}H_{l+1/2+v}^{-}((e^{-\nu r})^{A-1}\\ &\quad\times(1-e^{-\nu r})^{B+2}G_{l+1/2+v'})\,d\zeta\end{aligned} \tag{42}$$

since the operators $H_{l+1/2+v}^{\pm}$ are mutual adjoint. The following relations can easily be shown:

$$\begin{aligned}H_{l+1/2+v}^{-}&[(e^{-\nu r})^{A-1}(1-e^{-\nu r})^{B+2}]\\ &= [(e^{-\nu r})^{A-1}(1-e^{-\nu r})^{B+2}]\\ &\quad\times[-(A-1)\,e^{\nu r/2}(1-e^{-\nu r})+(B+2)\,e^{-\nu r/2}+H_{l+1/2+v}^{-}]\end{aligned} \tag{43a}$$

and

$$H_{l+1/2+v}^{-} = (v-v')\coth\zeta - \left(\frac{b+l(l+1)}{k+l} - \frac{b+l(l+1)}{k'+l}\right)\frac{1}{\sinh\zeta} + H_{l+1/2+v'}^{-}. \tag{43b}$$

Using (15) and ($43a, b$) we get

$$\begin{aligned}H_{l+1/2+v}^{-}&[(e^{-\nu r})^{A-1}(1-e^{-\nu r})^{B+2}]\\ &= [(e^{-\nu r})^{A-1}(1-e^{-\nu r})^{B+2}]\Big\{(e^{-\nu r})^{-1/2}(1-e^{-\nu r})\Big[-A-B-1+\tfrac{1}{2}(v-v')\\ &\quad+\frac{1}{2}\left(\frac{b+l(l+1)}{k+l}-\frac{b+l(l+1)}{k'+l}\right)\Big]+(e^{-\nu r})^{-1/2}(B+2+v'-v)+H_{l+1/2+v'}^{-}\Big\}.\end{aligned} \tag{44}$$

Inserting (44) into (42), we obtain

$$\begin{aligned}\mathcal{N}_{v,v'}^{A,B} &= [v(2l+v+1)]^{-1/2}\Big\{[v'(2l+v'+1)]^{1/2}\mathcal{N}_{v-1,v'-1}^{A,B}+(B+2+v'-v)\mathcal{N}_{v-1,v'}^{A-1/2,B}\\ &\quad+\Big[-A-B-1+\tfrac{1}{2}(v-v')+\frac{1}{2}\left(\frac{b+l(l+1)}{k+l}-\frac{b+l(l+1)}{k'+l}\right)\Big]\mathcal{N}_{v-1,v'}^{A-1/2,B+1}\Big\}.\end{aligned} \tag{45}$$

If we let $\nu \to 0$ in the recurrence formula (45) we get exactly the same expression as was found by Badawi *et al* (1973) for the hydrogen atom.

The recurrence formula (45) and its counterpart, obtained by formally interchanging k, v and k', v', are, together with formulae (36) and (39), all that is necessary for calculating any matrix element (14).

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