Spectrum of potentials $gr^{-(s+2)}$ via SL(2,R) acting on quaternions

1980 J. Phys. A: Math. Gen. 13 1243

(http://iopscience.iop.org/0305-4470/13/4/018)

J. Phys. A: Math. Gen. **13** (1980) 1243–1257. Printed in Great Britain

Spectrum of potentials $gr^{-(s+2)}$ via SL (2, $\mathbb{R}$) acting on quaternions

M Cl Dumont-Lepage†, N Gani‡, J P Gazeau§ and A Ronveaux†

† Département de physique, Facultés Universitaires, Notre-Dame de la Paix, B-5000 Namur, Belgium

‡ UER Informatique, Université de Paris VII, F-75005 Paris, France

§ Laboratoire de Chimie-Physique, 11, rue Pierre et Marie Curie, F-75005 Paris, France

Received 23 July 1979

Abstract. Potentials of the $r^{-(s+2)}$ power type are studied as the superposition of Yukawa potentials. The SL(2, $\mathbb{R}$) group acting on the quadrivector impulsion considered as a quaternion generates a compact self-adjoint operator deduced from the Schrödinger operator by a Fourier–Fock transformation. The operator is approximated by finite rank operators and gives the spectrum of energy as a function of the coupling constant, the angular momentum and the exponent s.

1. Introduction

Solutions of the Schrödinger equation for a central potential $V(r)$, singular at the origin $r = 0$, have interested both mathematicians and physicists (Landau and Lifschitz 1966, Simon 1971a) for a long time. Mathematics is mainly concerned with self-adjointness properties of the differential operator, while physics has something to learn from the rather strange behaviour of the energy levels in the vicinity of the attractive r^{-2} potential.

In this paper we study the discrete spectrum of the Schrödinger operator $H_0 + V(r)$ for a central attractive potential of the inverse power type, written in the form

$$V(r) = -g/r^{s+2}, \qquad g > 0 \tag{1}$$

We first classify the different potentials according to their exponent s, and we follow Kato and Simon (Simon 1971b).

In the range $-2 < s < -\frac{1}{2}$ this potential is in the class $L^2 + (L^\infty)_\epsilon$ (Simon 1971b) (i.e. $\forall \epsilon$, $V(r) = V^1_\epsilon(r) + V^2_\epsilon(r)$ with $V^1_\epsilon(r) \in L^2$ and $\|V^2_\epsilon(r)\|_\infty < \epsilon$).

In the range $-\frac{1}{2} \leqslant s < 0$, $V(r)$ is in the class $R + (L^\infty)_\epsilon$ where the R condition is a Rollnick one (Simon 1971b):

$$\iint \frac{|V(\boldsymbol{r})|\ \ |V(\boldsymbol{r}')|}{|\boldsymbol{r} - \boldsymbol{r}'|^2}\, \mathrm{d}\boldsymbol{r}\, \mathrm{d}\boldsymbol{r}' < \infty. \tag{2}$$

We give tables and curves of the first energy levels as functions of the coupling constant g, the exponent s and the orbital quantum number l.

The technique uses a Sturmian approach already developed for a larger class of interactions (Gazeau and Maquet 1979). The Schrödinger operator is replaced by a

Sturmian operator, denoted by A_s, equivalent to $(H_0-E)^{-1/2}V(H_0-E)^{-1/2}$, and this operator is compact for $E\in\mathbb{C}-\mathbb{R}^+$ and $V\in R+(L^\infty)_\epsilon$.

After a Fourier–Fock transformation (Gazeau 1978, 1979), the algebraic nature of the transformed Sturmian operator is recognised as a linear superposition of representation operators of SL(2, $\mathbb{R}$). Two advantages emerge from this approach. First, the matrix elements of this operator are universal in the sense that once computed, superposition of potentials implies superposition of universal matrix elements. Besides, the projected operators $A_{s,l}$ on each l angular subspace are compact self-adjoint operators on appropriate Hilbert spaces and can therefore be approximated by finite rank operators.

Let us now begin the next section with a study of the projected Sturmian operator $A_{s,l}$.

2. SL(2, $\mathbb{R}$) Sturmian technique

The trick in this approach uses the exponential $e^{-\gamma r}$ in the Yukawa potential as a Laplace kernel. The potential is then, by superposition, the Laplace transform of a power.

Explicitly, the potential

$$V(r)=-g/r^{s+2} \tag{3}$$

is the Laplace transform

$$V(r)=\frac{-g}{\Gamma(s+1)}\int_0^\infty d\gamma\gamma^s\frac{e^{-\gamma r}}{r} \qquad (s>-1). \tag{4}$$

Let us first summarise the Fourier–Fock technique.

(i) The Fourier transform of the Schrödinger equation,

$$[-(\hbar^2/2m)\nabla^2-E]\psi(\boldsymbol{r})=-V(\boldsymbol{r})\psi(\boldsymbol{r}), \tag{5}$$

gives the following integral equation for the Fourier transform of the wavefunction (Bethe and Salpeter 1957):

$$(\|\boldsymbol{p}\|^2+p_0^2)\chi(\boldsymbol{p})=\frac{mg}{\pi^2\hbar\Gamma(s+1)}\int_0^\infty d\gamma\gamma^s\int d^3\boldsymbol{p}'V_\gamma(\boldsymbol{p},\boldsymbol{p}')\chi(\boldsymbol{p}'), \tag{6}$$

with

$$p_0=(-2\,mE)^{1/2} \qquad (E<0),$$

and where $\chi(\boldsymbol{p})$, $V_\gamma(\boldsymbol{p},\boldsymbol{p}')$ are the Fourier transforms of the wavefunction $\psi(\boldsymbol{r})$ and the elementary potential $e^{-\gamma r}/r$ respectively.

$$\chi(\boldsymbol{p})=\frac{1}{(2\pi)^{3/2}}\int d^3\boldsymbol{r}\,\psi(\boldsymbol{r})\exp\left(-\frac{i}{\hbar}\boldsymbol{p}\boldsymbol{r}\right) \tag{7}$$

$$V_\gamma(\boldsymbol{p},\boldsymbol{p}')=(\|\boldsymbol{p}-\boldsymbol{p}'\|^2+\gamma^2\hbar^2)^{-1}.$$

(ii) Group theory can be applied to the $\boldsymbol{p}$ integral equation after the introduction of the quaternionic field and a stereographic projection as in the Fock technique.

Let us first identify the four-vector $(p_0, \boldsymbol{p}) \equiv (p_0, p_1, p_2, p_3)$ with the quaternion x written in matrix form as

$$x = \begin{pmatrix} p_0 + ip_1 & -p_3 + ip_2 \\ p_3 + ip_2 & p_0 - ip_1 \end{pmatrix}, \tag{8}$$

with norm $|x|^2 = p_0^2 + \|\boldsymbol{p}\|^2$.

Now we map the quaternion x onto the point ξ belonging to the S_3 sphere (SU(2) manifold or quaternion of unit norm) via the stereographic projection

$$\xi \equiv s^{-1}(p_0) \cdot x = x(2p_0 - x)^{-1} = x\bar{x}^{-1}, \tag{9}$$

where $\bar{x} \equiv (p_0, -\boldsymbol{p})$.

It follows that

$$|\xi|^2 = \xi_0^2 + \|\boldsymbol{\xi}\|^2 = 1, \tag{10}$$

with

$$\xi_0 = \frac{p_0^2 - \|\boldsymbol{p}\|^2}{|x|^2}, \qquad \boldsymbol{\xi} = \frac{2p_0}{|x|^2}\boldsymbol{p}. \tag{11}$$

This quaternionic transformation is a homographic one belonging to the group SL $(2, \mathbb{R})$ acting as conformal transformation on $\mathbb{H}$†:

$$s^{-1}(p_0) = \frac{1}{(2p_0)^{1/2}} \begin{pmatrix} 1 & 0 \\ -1 & 2p_0 \end{pmatrix}, \tag{12}$$

$$x' \equiv g.x = (ax + b)(cx + d)^{-1} \begin{cases} g = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \\ ad - bc = 1 \end{cases} \tag{13}$$

This one-to-one mapping sends the hyperplane (p_0 fixed) onto the three-dimensional unit sphere, and as usual the point at infinity goes to the South pole (see figure 1).

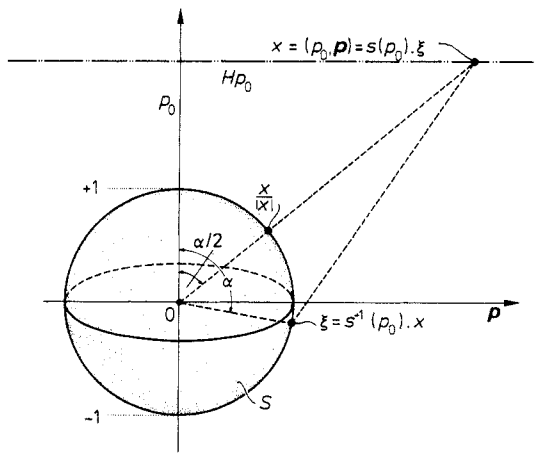

Figure 1. Quaternion mapping.

† We identify any real number a with the quaternion $(a, \mathbf{0})$.

With each function $\chi(p_0, \boldsymbol{p}) \equiv \chi(\boldsymbol{p})$ which is square integrable on the hyperplane H_{p_0}, the Fock transformation $\mathscr{F}_{p_0}$ associates a function on the SU(2) manifold. The correspondence is given explicitly by

$$(\mathscr{F}_{p_0}\chi)(\xi) \equiv \phi_{p_0}(\xi) = \frac{1}{\sqrt{p_0}}\left(\frac{2p_0}{|1+\xi|^2}\right)^2 \chi(s(p_0).\xi) \tag{14}$$

or

$$(\mathscr{F}_{p_0}^{-1}\phi)(x) = \sqrt{p_0}\,(2p_0/|x|^2)^2 \phi_{p_0}(s^{-1}(p_0).x). \tag{15}$$

In the inverse transformation we use the property

$$|1+\xi|^2 = 4p_0^2/|x|^2. \tag{16}$$

(iii) The integral equation in the H_{p_0} hyperplane now becomes an integral equation on the SU(2) manifold via the stereographic transformation.

(a) The Euclidean three-dimensional measure is transformed in the following way:

$$[(2p_0)^3/|x|^6]\,\mathrm{d}\boldsymbol{p} = \mathrm{d}\mu(\xi) = \sin^2\alpha\,\sin\theta\,\mathrm{d}\alpha\,\mathrm{d}\theta\,\mathrm{d}\phi \tag{17}$$

where (α, θ, ϕ) are spherical coordinates of the unit quaternion ξ on the SU(2) manifold.

The inner product in $F_{p_0} \equiv L^2_{\mathbb{C}}$ $(H_{p_0} \simeq (R^3))$ is $\mathscr{F}_{p_0}$, related to the inner product on $E_{p_0} \equiv L^2_{\mathbb{C}}$ (SU(2)) by

$$\int \mathrm{d}\boldsymbol{p}\chi(p_0, \boldsymbol{p})\chi'^{*}(p_0, \boldsymbol{p}) \equiv (\chi, \chi')_{F_{p_0}} = \tfrac{1}{2}(|1+\xi|^2\phi_{p_0}, \phi'_{p_0})_{E_{p_0}} \tag{18}$$

and

$$\int \mathrm{d}\mu(\xi)\phi_{p_0}(\xi)\phi'^{*}_{p_0}(\xi) \equiv (\phi_{p_0}, \phi'_{p_0})_{E_{p_0}} = (1/2p_0^2)(|x|^2\chi, \chi')_{F_{p_0}} \equiv (\chi, \chi')_{F_{p_0+1}}, \tag{19}$$

where

$$\phi_{p_0} = \mathscr{F}_{p_0}\chi, \qquad \phi'_{p_0} = \mathscr{F}_{p_0}\chi'$$

and where F_{p_0+1} is the first Sobolev space, i.e. the Hilbert space with the inner product $(\chi, \chi')_{F_{p_0+1}}$.

The linear transformation $\mathscr{F}_{p_0}$ is thus an isomorphism between the spaces F_{p_0+1} and E_{p_0}.

(b) The homographic action on the kernel gives the result

$$\begin{aligned}(\|\boldsymbol{p}-\boldsymbol{p}'\|^2 + \gamma^2\hbar^2)^{-1} &= |(p_0, \boldsymbol{p}') - (p_0 - \gamma\hbar, \boldsymbol{p})|^{-2} \\ &= \frac{4p_0^2}{|x|^2|x'|^2}\,|\beta\xi + 1 + \beta|^{-2}|\xi' - g^{-1}(\beta).\xi|^{-2}\end{aligned} \tag{20}$$

where

$$\beta = \gamma\hbar/2p_0,$$

$$g^{-1}(\beta) = g(-\beta) = s^{-1}(p_0)t_{-\gamma\hbar}s(p_0) = \begin{pmatrix} 1-\beta & -\beta \\ \beta & 1+\beta \end{pmatrix} \in \mathrm{SL}(2, \mathbb{R}), \tag{21}$$

with

$$t_{-\gamma\hbar} = \begin{pmatrix} 1 & -\gamma\hbar \\ 0 & 1 \end{pmatrix}.$$

(iv) The Schrödinger equation is therefore transformed into an eigenvalue problem for the operator A_s:

$$(I - \nu A_s)\phi_{p_0} = 0 \qquad (\phi_{p_0} \in E_{p_0}) \tag{22}$$

with $\nu = mg/p_0\hbar$,

$$\begin{aligned} A_s\phi_{p_0}(\xi) &\equiv \left(\frac{2p_0}{\hbar}\right)^{s+1} \frac{1}{2\pi^2\Gamma(s+1)} \\ &\quad \times \int_0^\infty d\beta\beta^s \int d\mu(\xi')|\xi\beta + 1 + \beta|^{-2}|\xi' - g^{-1}(\beta)\xi|^{-2}\phi(\xi') \\ &\equiv \left(\frac{2p_0}{\hbar}\right)^{s+1} \frac{1}{4\pi\Gamma(s+1)\cos s\pi/2} \int d\mu\ (\xi') \frac{|\xi - \xi'|^{s-1}}{|1+\xi|^{s+1}|1+\xi'|^{s+1}} \phi(\xi'). \end{aligned} \tag{23}$$

This integral operator is compact, self-adjoint and positive. The Poisson kernel in $\mathbb{R}^4$ appears in the computation of the last term:

$$|\xi' - g^{-1}(\beta).\xi|^{-2} = \int_0^\infty dt\, e^{-t} \frac{1 - e^{-t}|g^{-1}(\beta)\,.\,\beta|^2}{|\xi' - e^{-t}g^{-1}(\beta)\,.\,\xi|^4}, \tag{24}$$

and the multiplication of a quaternion by e^{-t} is equivalent to the contracting conformal action

$$\delta(-t) = \begin{pmatrix} e^{-t/2} & 0 \\ 0 & e^{t/2} \end{pmatrix}. \tag{25}$$

The Sturmian operator A_s is now written in terms of group representation operators:

$$A_s = \frac{1}{\Gamma(s+1)} \left(\frac{2p_0}{\hbar}\right)^{s+1} \int_0^\infty d\beta\, \beta^s \int_0^\infty dt\, \mathscr{C}(g(\beta)\delta(t)) \tag{26}$$

where $\mathscr{C}$ is a local representation of $SL(2, \mathbb{R})$ on E_{p_0} defined by

$$\mathscr{C}(g)\phi(\xi) = \frac{1}{2\pi_2}|c\xi + d|^{-2} \int_{SU(2)} d\mu(\xi')\phi(\xi') \frac{1 - |g^{-1}\,.\,\xi|^2}{|\xi' - g^{-1}\,.\,\xi|^4}, \tag{27}$$

with

$$g^{-1} = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in SL(2, \mathbb{R}).$$

The matrix elements of this representation with respect to the hyperspherical harmonics $Y_{nlm}(\xi)$ (Gazeau 1978, 1979), $n > l$, $|m| \leq l$ (Coulomb Sturmian basis) are given by

$$\begin{aligned} \mathscr{C}_{nlm,n'l'm'}(g) &\equiv (\mathscr{C}(g)\, Y_{n'l'm'},\ Y_{nlm}) \\ &= \delta_{ll'}\delta_{mm'} \left(\frac{n'}{n}\right)^{1/2} \left(\frac{(n_> - l - 1)!(n_> + l)!}{(n_< - l - 1)!(n_< + l)!}\right)^{1/2} d^{-(n_> + l + 1)} a^{n_< - l - 1} \frac{\gamma(b, c)^{n_> - n_<}}{(n_> - n_<)!} \\ &\quad \times {}_2F_1(l + 1 - n_<,\ n_> + l + 1;\ n_> - n_< + 1;\ bc/ad) \end{aligned} \tag{28}$$

where

$$n_<^> = \begin{cases} \sup \\ \inf \end{cases} (n, n')$$

$$\gamma(b, c) = \begin{cases} b \text{ if } n_> = n' \\ -c \text{ if } n_> = n. \end{cases}$$

Let us now separate the variables on the S^3 sphere into the hyperspherical form

$$\phi(\xi) = a_l(\alpha)\sin^l\alpha\, Y_{lm}(\theta, \phi), \tag{29}$$

where Y_{lm} are the usual spherical harmonics. The initial eigenvalue problem then becomes

$$(I - \nu A_{s,l})a_l(\alpha) = 0. \tag{30}$$

The operator $A_{s,l}$ now acts on the Hilbert space of functions $a_l(\alpha)$ satisfying

$$\int_0^\pi \mathrm{d}\alpha\,(\sin\alpha)^{2l+1}|a_l(\alpha)|^2 < \infty. \tag{31}$$

From equation (26), this projected operator is also a linear superposition of local representation operators T^{l+1} of $\mathrm{SL}(2, \mathbb{R})$.

The matrix elements of this operator in the orthonormal basis of Gegenbauer polynomials $N_{i,l}C_{i-1}^{l+1}(\cos\alpha)$ ($i = n - l > 0$; $N_{i,l}$ are normalisation constants) are given by

$$\begin{aligned}(A_{s,l})_{i,i'} = {} & \frac{1}{\Gamma(s+1)}\left(\frac{2p_0}{\hbar}\right)^{s+1}\left(\frac{i'+l}{i+l}\right)^{1/2}\left(\frac{(i_>-1)!(i_>+2l)!}{(i_<-1)!(i_<+2l)!}\right)^{1/2}\frac{(-1)^{i_>-i_<}}{(i_>-i_<)!} \\ & \times\left(\int_0^\infty \mathrm{d}\beta\left\{\beta^{s+i_>-i_<}(1+\beta)^{-(i_>+2l+1)}(1-\beta)^{i_<-1}\right.\right. \\ & \left.\left.\times {}_2F_1[1-i_<, i_>+2l+1; i_>-i_<+1; \beta^2/(\beta^2-1)]\right\}\int_0^\infty \mathrm{d}t\,\exp[-(i'+l)t]\right).\end{aligned} \tag{32}$$

Let us note that

$$(A_{s,l})_{i,j} = (2p_0/\hbar)^{s+1}\Lambda_{i,j}(s, l) \qquad (i, j > 0). \tag{33}$$

The numerical matrix elements $\Lambda_{i,j}(s, l)$ are then given after a trivial integration with respect to β by

$$\begin{aligned}\underset{i\leqslant j}{\Lambda_{i,j}}(s, l) = {} & \Gamma(2l+1-s)\frac{(-1)^{i+j}}{[(i+l)(j+l)]^{1/2}}\left[\frac{(i-1)!(j-1)!}{(i+2l)!(j+2l)!}\right]^{1/2} \\ & \times\sum_{\sigma=1}^{i}\left(\frac{(2l+1-s)_{\sigma-1}}{(\sigma-1)!}\frac{(s+1)_{i-\sigma}}{(i-\sigma)!}\frac{(s+1)_{j-\sigma}}{(j-\sigma)!}\right)\end{aligned} \tag{34}$$

where

$$(a)_n = \frac{\Gamma(a+n)}{\Gamma(a)} \qquad \text{(Pochhammer symbol)},$$

the matrix $\Lambda \equiv (\Lambda_{i,j}(s, l))$ being symmetric.

(v) Let $\lambda_q(s, l)$ be the qth eigenvalue of the infinite symmetric matrix Λ, and $\nu_q(s, l)$ the inverse of the qth eigenvalue of the operator $A_{s,l}$; then $\lambda_q(s, l)$ and $\nu_q(s, l)$ are obviously connected by the relation

$$\nu_q(s, l)\left(\frac{2(-2mE_q)^{1/2}}{\hbar}\right)^{s+1} = (\lambda_q(s, l))^{-1}. \tag{35}$$

Let us avoid dimensionality problems by defining first

$$g = g'L^s, \qquad K = 2mg'/\hbar^2, \tag{36}$$

and choosing the units such that (Rydberg units)

$$\hbar^2/8\, mL^2 = 1; \tag{37}$$

the energy levels (numbered by q) are finally given by

$$E_q(s, l) = -(K\lambda_q(s, l))^{-2/s}. \tag{38}$$

3. Numerical results

In order to draw the curves $E_q(s, l)$ for fixed l, in the interval $-2 < s < 0$ the eigenvalues $\lambda_q(s, l)$ were computed on a computer DIGITAL DEC system 2050. The program was written in FORTRAN using the subroutine EIGEN of IBM, which gives the eigenvalues (and the eigenvectors on request) of a real symmetric matrix. Since the infinite matrices $\Lambda(s, l)$ are compact, they can be approximated by finite rank matrices. The approximations of order f, $\Lambda^{(f)}(s, l)$ are obtained by selecting the first f rows and columns of the original matrices. The spectrum of $\Lambda^{(f)}(s, l)$ is denoted by $\lambda_q^{(f)}(s, l)$ and the sequence $(\lambda_q^{(f)}(s, l)_{q \leqslant f}$ must converge to the required value $\lambda_q(s, l)$. The rate of convergence is good in the interval $-2 < s < -0{\cdot}5$, but in the range $-0{\cdot}5 \leqslant s < 0$ the slow convergence has been accelerated by the Aitken Δ^2 process (Brezinski 1977). It is interesting to notice that in that range the potential loses the L^2 character $L^2 + L_\epsilon^\infty$ as indicated in the Introduction. In the Coulomb case ($s = -1$) all truncated eigenvalues give the exact value for the Coulomb levels:

$$\begin{aligned} &\lambda_q(-1, l) = 1/(q + l), \\ &E_q(-1, l) = K^2/(q + l)^2. \end{aligned} \tag{39}$$

When $s = -2$ the symmetric Λ matrix takes a tridiagonal form, and its elements are defined by

$$\begin{cases} \Lambda_{ii}(-2, l) = 2, \\ \Lambda_{i,i+1}(-2, l) = \Lambda_{i+1,i}(-2, l) = \left(\dfrac{i(2l + i + 1)}{(i + l)(i + l + 1)}\right)^{1/2}. \end{cases} \tag{40}$$

It is now the matrix of a non-compact operator owning a continuous spectrum. In the $l = 0$ case the $\Lambda_{ij}(-2, 0)$ are 2 (if $i = j$), 1 (if $i = j + 1$ or $i = j - 1$) or 0 (otherwise), and it is easily shown (Wilf 1970) that the spectrum is the interval $[0, 4]$. Then, from the behaviour of the $\nu_q(s, 0)$ in the neighbourhood of $s = -2$ (see figure 2) it can be deduced that

$$E_q(s, 0)_{s \to -2} \to -4K, \qquad \forall q = 1, 2, \ldots. \tag{41}$$

Now, we notice the absence of crossing of energy levels in the neighbourhood of $s = -2$ (see figure 5 or figure 6) and therefore the energy levels take the same value for all angular momentum l, i.e.

$$E_q(s, l)_{s \to -2} \to -4K \qquad \begin{cases} \forall\, l = 0, 1, \ldots \\ \forall\, q = 1, 2, \ldots. \end{cases} \tag{42}$$

It follows that

$$\lambda_q(s, l)_{s \to -2} \to 4. \tag{43}$$

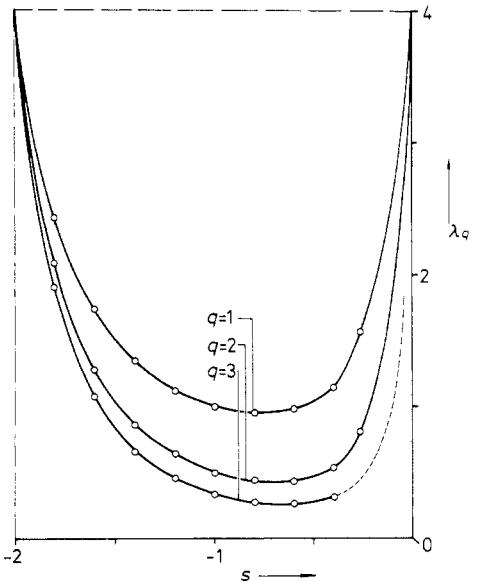

Figure 2. Eigenvalues $\lambda_q(s, 0)$; $q = 1, 2, 3$; $l = 0$.

In the $s = 0$ case, expression (34) becomes

$$\Lambda_{\substack{i,j \\ i\leqslant j}}(0, l) = \frac{1}{2l+1}\frac{(-1)^{i+j}}{[(i+l)(j+l)]^{1/2}}\left(\frac{(2l+i)!(j-1)!}{(2l+j)!(i-1)!}\right)^{1/2}. \tag{44}$$

The matrix elements are those of a non-compact operator, the spectrum of which is included in the interval $(0, 4)$ if $l = 0$. Schwartz (1976) showed that when s is close to zero the eigenvalues have the following behaviour:

$$\lambda_q(s, l) \underset{s\gtrless 0}{\approx} \left(\frac{1}{2L}\right)^{-s}\frac{4}{Z_q^2 s^2}, \qquad \begin{cases} q = 1, 2, \ldots \\ l = 0, 1, \ldots \end{cases} \tag{45}$$

where Z_q is the qth zero of the Bessel function $J_\nu(x)$ of order $\nu = (2l+1)/s$. It follows that at the limit point $s = 0$, the $\lambda_q(s, l)$ (for fixed l) converge to the same value:

$$\lambda^*(0, l) = 4/(2l+1)^2. \tag{46}$$

Thus there exists for each l a critical value of the coupling constant g (and thus of K) denoted by g_l^* (K_l^*) which drastically modifies the behaviour of the energy levels:

$$g_l^* = L^2(2l+1)^2, \qquad K_l^* = (2l+1)^2/4, \tag{47}$$

and

$$\begin{aligned} &E_q(s, l) \underset{s\gtrless 0}{\longrightarrow} 0, \qquad \forall q = 1, 2, \ldots \text{ and } \forall g < g_l^* \\ &E_q(s, l) \underset{s\gtrless 0}{\longrightarrow} -\infty, \qquad \forall q = 1, 2, \ldots \text{ and } \forall g > g_l^*. \end{aligned} \tag{48}$$

Table 1 shows the rate of convergence of the eigenvalues $\lambda_q^{(f)}(s, l)$ of the truncated operators $\Lambda^f(s, l)$. We show explicitly only the convergence of the first three levels in the $l = 0$ case for three typical values of the exponents.

Table 1. Convergence of the eigenvalues $\lambda_q^{(f)}(s, l)$ to $\lambda_q(s, l)$. (*a*) $s = -1{\cdot}8$, $l = 0$, (*b*) $s = -1{\cdot}2$, $l = 0$; (*c*) $s = -0{\cdot}4$, $l = 0$.

Table 1(*a*).

f	$q=1$	$q=2$	$q=3$
10	2·433 31	2·077 22	1·883 37
15	2·433 31	2·077 65	1·903 13
20	2·433 31	2·077 65	1·903 23
25	2·433 31	2·077 65	1·903 23

Table 1(*b*).

f	$q=1$	$q=2$	$q=3$
2	1·125 67	0·593 13	
4	1·125 95	0·629 34	0·449 90
6	1·125 97	0·629 40	0·450 58
8	1·125 98	0·629 41	0·450 59
10	1·125 98	0·629 42	0·450 60
⋮	⋮	⋮	⋮
30	1·125 99	0·629 43	0·450 61

Table 1(*c*).

f	$q=1$	$q=2$	$q=3$
15	1·131 37	0·472 80	0·248 21
20	1·135 28	0·484 10	0·260 59
25	1·137 39	0·490 95	0·268 75
30	1·138 68	0·495 50	0·274 55
35	1·139 52	0·498 70	0·278 89
60	1·141 31	0·506 33	0·290 51
Δ^2	1·141 89	0·509 92	0·298 34

Table 2 gives the eigenvalues $\lambda_q(s, l)$ of the operator $\Lambda(s, l)$. The interval $-2 < s < 0$ is covered with nine points. The first three levels are given for an angular momentum l ranging from 0 to 4.

Table 2. Eigenvalues $\lambda_q(s, l)$ of the operator $\Lambda(s, l)$.

	q \ s	-2	$-1{\cdot}8$	$-1{\cdot}6$	$-1{\cdot}4$	$-1{\cdot}2$
	1		2·4333	1·7432	1·3543	1·1260
$l=0$	2	$\lambda_{max}=4$	2·0776	1·2792	0·8619	0·6294
	3		1·9032	1·0756	0·6672	0·4506
	1		2·1534	1·3564	0·9192	0·6601
$l=1$	2	$\lambda_{max}=4$	1·9504	1·1205	0·6986	0·4665
	3		1·8246	0·9838	0·5781	0·3660
	1		1·9967	1·1635	0·7275	0·4804
$l=2$	2	$\lambda_{max}=4$	1·8577	1·0131	0·5970	0·3749
	3		1·7608	0·9132	0·5140	0·3100
	1		1·8904	1·0417	0·6150	0·3829
$l=3$	2	$\lambda_{max}=4$	1·7860	0·9344	0·5270	0·3157
	3		1·7079	0·8572	0·4657	0·2700
	1		1·8110	0·9553	0·5394	0·3209
$l=4$	2	$\lambda_{max}=4$	1·7280	0·8736	0·4752	0·2740
	3		1·6630	0·8115	0·4277	0·2400

Table 2—continued.

	q \ s	−1·0	−0·8	−0·6	−0·4	−0·2	0
	1	1·0000	0·9534	0·9881	1·142	1·57	
$l=0$	2	0·5000	0·4379	0·434	0·51	0·8	$\lambda_{max}=4$
	3	0·3333	0·2748	0·261	0·3		
	1	0·5000	0·3998	0·3394	0·310	0·315	
$l=1$	2	0·3333	0·2562	0·214	0·201	0·22	$\lambda_{max}=0·4444$
	3	0·2500	0·1858	0·153	0·145		
	1	0·3333	0·2429	0·1868	0·1531	0·1374	
$l=2$	2	0·2500	0·1776	0·1355	0·1133	0·108	$\lambda_{max}=0·1600$
	3	0·2000	0·1388	0·1050	0·0889		
	1	0·2500	0·1710	0·1231	0·094 01	0·078 05	
$l=3$	2	0·2000	0·1342	0·096 14	0·0746	0·0652	$\lambda_{max}=0·081\,63$
	3	0·1667	0·1099	0·078 27	0·0614	0·057	
	1	0·2000	0·1304	0·089 30	0·064 74	0·050 82	
$l=4$	2	0·1667	0·1071	0·073 04	0·0536	0·0438	$\lambda_{max}=0·049\,38$
	3	0·1428	0·090 47	0·061 47	0·0456	0·038	

The corresponding energy levels are tabulated in Rydberg units for the constant $K=1$ in table 3 and in table 4 when $K=10$.

The eigenvalues $\lambda_q(s, l)$ are also plotted in figure 2 ($l=0$), figure 3 ($l=1$), and figure 4 ($l=2$) ($q=1, 2, 3$). The energy levels are plotted in figure 5 when $K=1$ and $l=0, 1$ and figure 6 shows the levels when $K=10$ and $l=0, 1, 2$.

Table 3. Energy levels for the value of the parameter $K=2mg'/\hbar^2=1$.

	q \ s	−2	−1·8	−1·6	−1·4	−1·2	−1·0
	1	−4	−2·686	−2·003	−1·542	−1·218	−1·000
$l=0$	2	−4	−2·253	−1·360	−0·809	−0·462	−0·250
$K^*=0·25$	3	−4	−2·044	−1·095	−0·561	−0·265	−0·111
	1	−4	−2·345	−1·464	−0·887	−0·500	−0·250
$l=1$	2	−4	−2·101	−1·153	−0·599	−0·281	−0·111
$K^*=2·25$	3	−4	−1·951	−0·980	−0·457	−0·187	−0·0625
	1	−4	−2·156	−1·208	−0·635	−0·295	−0·111
$l=2$	2	−4	−1·990	−1·016	−0·479	−0·195	−0·625
$K^*=6·25$	3	−4	−1·875	−0·893	−0·386	−0·142	−0·0400
	1	−4	−2·029	−1·052	−0·499	−0·202	−0·0625
$l=3$	2	−4	−1·905	−0·919	−0·400	−0·146	−0·0400
$K^*=12·25$	3	−4	−1·812	−0·825	−0·336	−0·113	−0·0278
	1	−4	−1·934	−0·944	−0·414	−0·150	−0·0400
$l=4$	2	−4	−1·836	−0·845	−0·345	−0·115	−0·0278
$K^*=20·25$	3	−4	−1·760	−0·770	−0·297	−0·0926	−0·0204

Table 3—continued.

	q \ s	−0·8	−0·6	−0·4	−0·2	0
$l=0$ $K^*=0{\cdot}25$	1	−0·887	−0·961	−1·942	$-9{\cdot}1\times10$	$-\infty$
	2	−0·127	$-0{\cdot}619\times10^{-1}$	$-0{\cdot}34\times10^{-1}$	−0·1	$-\infty$
	3	−0·0396	$-0{\cdot}114\times10^{-1}$	$-0{\cdot}2\times10^{-2}$		$-\infty$
$l=1$ $K^*=2{\cdot}25$	1	−0·101	$-0{\cdot}273\times10^{-1}$	$-0{\cdot}286\times10^{-2}$	$-0{\cdot}96\times10^{-5}$	0
	2	−0·0332	$-0{\cdot}586\times10^{-2}$	$-0{\cdot}328\times10^{-3}$	$-0{\cdot}26\times10^{-6}$	0
	3	−0·0149	$-0{\cdot}191\times10^{-2}$	$-0{\cdot}641\times10^{-4}$		0
$l=2$ $K^*=6{\cdot}25$	1	−0·0291	$-0{\cdot}373\times10^{-2}$	$-0{\cdot}841\times10^{-4}$	$-0{\cdot}240\times10^{-8}$	0
	2	−0·0133	$-0{\cdot}128\times10^{-2}$	$-0{\cdot}187\times10^{-4}$	$-0{\cdot}216\times10^{-9}$	0
	3	−0·007 18	$-0{\cdot}546\times10^{-3}$	$-0{\cdot}552\times10^{-5}$		0
$l=3$ $K^*=12{\cdot}25$	1	−0·0121	$-0{\cdot}928\times10^{-3}$	$-0{\cdot}734\times10^{-5}$	$-0{\cdot}839\times10^{-11}$	0
	2	−0·0661	$-0{\cdot}407\times10^{-3}$	$-0{\cdot}231\times10^{-5}$	$-0{\cdot}139\times10^{-11}$	0
	3	−0·0401	$-0{\cdot}205\times10^{-3}$	$-0{\cdot}873\times10^{-6}$	$-0{\cdot}36\times10^{-12}$	0
$l=4$ $K^*=20{\cdot}25$	1	−0·0614	$-0{\cdot}318\times10^{-3}$	$-0{\cdot}114\times10^{-5}$	$-0{\cdot}114\times10^{-12}$	0
	2	−0·0375	$-0{\cdot}163\times10^{-3}$	$-0{\cdot}442\times10^{-6}$	$-0{\cdot}260\times10^{-13}$	0
	3	−0·0246	$-0{\cdot}917\times10^{-4}$	$-0{\cdot}197\times10^{-6}$	$-0{\cdot}6\times10^{-14}$	0

Table 4. Energy levels for the value of the parameter $K=2mg'/\hbar^2=10$.

	q \ s	−2	−1·8	−1·6	−1·4	−1·2
$l=0$	1	−40	−34·69	−35·62	−41·38	−56·56
	2	−40	−29·10	−24·19	−21·70	−21·46
	3	−40	−26·40	−19·48	−15·05	−12·29
$l=1$	1	−40	−30·29	−26·03	−23·79	−23·23
	2	−40	−27·13	−20·50	−16·07	−13·03
	3	−40	−25·20	−17·42	−12·26	−8·69
$l=2$	1	−40	−27·85	−21·48	−17·03	−13·68
	2	−40	−25·70	−18·07	−12·84	−9·05
	3	−40	−24·22	−15·87	−10·37	−6·59

	q \ s	−1·0	−0·8	−0·6	−0·4	−0·2	0
$l=0$	1	−10·00	−2807	−2070	$-1{\cdot}942\times10^{5}$	$-9{\cdot}1\times10^{11}$	$-\infty$
	2	−25·00	−40·11	−133·3	$-3{\cdot}4\times10^{3}$	$-0{\cdot}1\times10^{10}$	$-\infty$
	3	−11·11	−12·51	−24·5	$-0{\cdot}2\times10^{3}$		$-\infty$
$l=1$	1	−25·00	−31·96	−58·75	$-2{\cdot}86\times10^{2}$	$-0{\cdot}96\times10^{5}$	$-\infty$
	2	−11·11	−10·50	−12·6	$-3{\cdot}28\times10$	$-0{\cdot}26\times10^{4}$	$-\infty$
	3	−6·25	−47·05	−4·13	−6·41	–	$-\infty$
$l=2$	1	−11·11	−9·19	−8·03	$-0{\cdot}841\times10$	$-0{\cdot}240\times10^{2}$	$-\infty$
	2	−6·25	−4·20	−2·75	$-0{\cdot}187\times10$	$-0{\cdot}216\times10$	$-\infty$
	3	−4·00	−2·27	−1·18	$-0{\cdot}552\times10$		$-\infty$

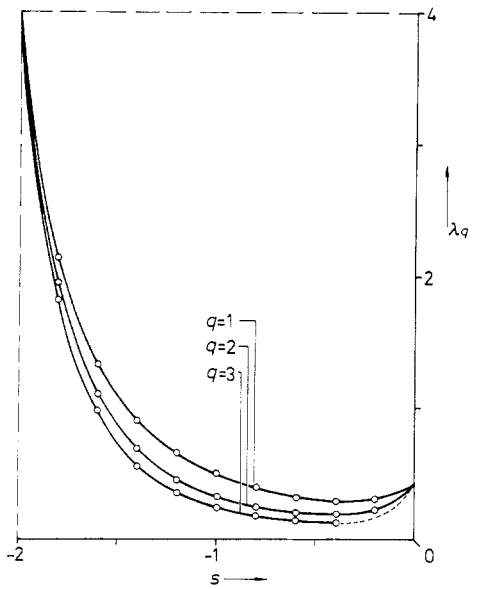

Figure 3. Eigenvalues $\lambda_q(s, 1)$; $q = 1, 2, 3$; $l = 1$.

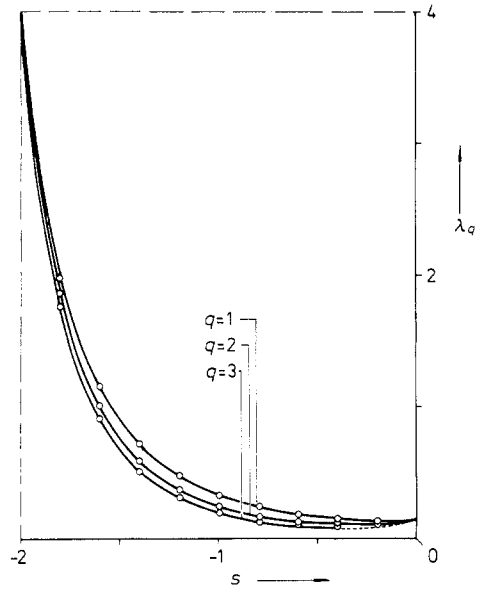

Figure 4. Eigenvalues $\lambda_q(s, 2)$; $q = 1, 2, 3$; $l = 2$.

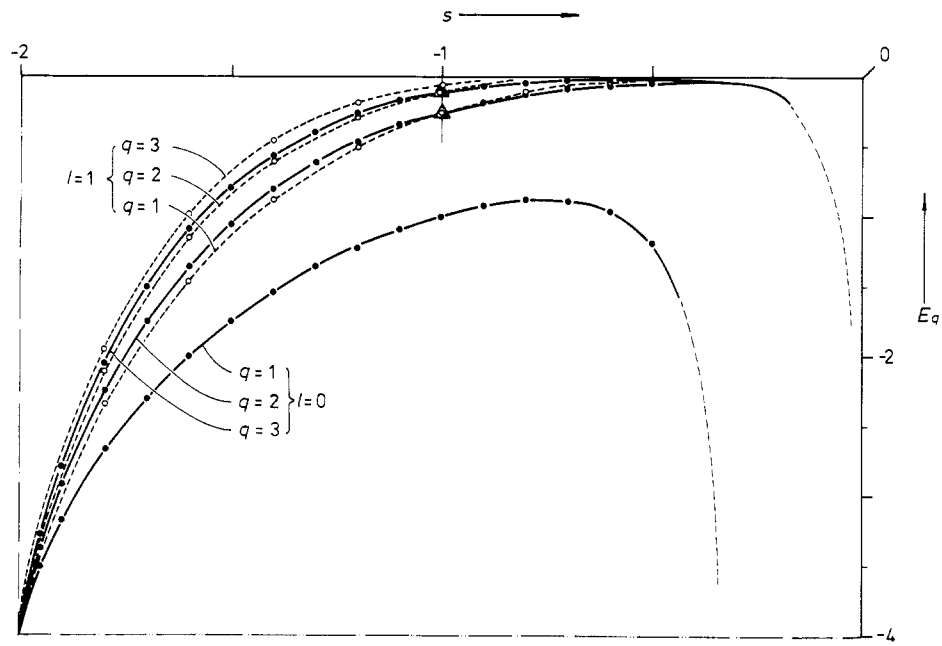

Figure 5. Energy levels $E_q(s, l)$; $q = 1, 2, 3$; $l = 0, 1$; $K = 1$.

4. Comparison with other works

Variational calculation has been applied in several ways in order to obtain the ground state of the inverse power potential $-g/r^{s+2}$ $(g > 0)$.

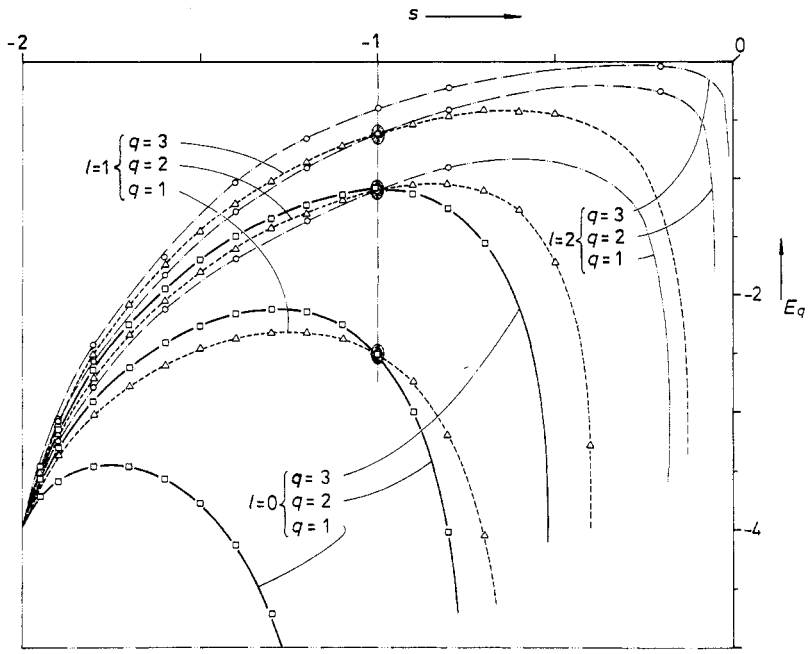

Figure 6. Energy levels $E_q(s, l)$; $q = 1, 2, 3$; $l = 0, 1, 2$; $K = 10$.

Baumgartner (1979), starting from the Schwartz inequality, gives the following expression as a lower bound for the ground state $l = 0$ ($\hbar^2 = 2m = 1$; $-2 < s < -1$, $g = 1$):

$$E_0 \geqslant s\left(\frac{s+2}{2}\right)^{(s+2)/|s|}. \tag{49}$$

Duchon (private communication) also uses a variational principle starting from the Sobolev inequality (Sobolev 1938) and gives, in the full interval $-2 < s < 0$, the following expression ($\hbar^2 = 2m = 1$):

$$E_0 \geqslant -3\left\{\frac{g}{3}\left[\frac{8}{\pi}\beta\left(\frac{3}{s+2} - \frac{3}{2}, \frac{3}{2}\right)\right]^{(s+2)/3}\right\}^{-2/s}. \tag{50}$$

In table 5 we compare our numerical results with the bounds given by these two authors.

Table 5. Ground state energy. Exact versus lower bounds ($g = 1$) ($\hbar^2 = 2m = 1$).

E_0 \ s	−2	−1·75	−1·5	−1·25	−1·0	−0·7	−0·5	−0·4
Our	−1	−0·6214	−0·4380	−0·3223	−0·2500	−0·2220	−0·2985	−0·486
Duchon	−1	−0·66	−0·49	−0·39	−0·33	−0·35	−0·59	−1·22
Baumgartner	−1	−0·6501	−0·4725	−0·3470	−0·2500			

5. Conclusions

The analytic solution of the Schrödinger equation for the attractive inverse power potential is not known, except of course in the Coulomb case. It was shown, some time ago, that for the potential $V(r) = gr^{-1/2}$ the Schrödinger equation can be solved in terms of some Heun confluent functions (Lemieux and Bose 1969), but eigenvalues and exact eigenfunctions have, apparently, not yet been published (Decarreau *et al* 1978).

In this work we give solutions of this problem, using a group approach, starting from a Sturmian formulation of the Schrödinger equation. The numerical part appears only at the final step, when the compact operator is approximated by finite Hermitian matrices. However, we insist on the fact that the given matrix elements are known exactly, and therefore we consider our approach as an analytic one. Let us still insist on the fact that this technique applies only to 'regular potentials' (Landau and Lifschitz 1966, Simon 1971a) $V(r)$ such that

$$\begin{cases} r^2 V(r) \xrightarrow[r\to 0]{} 0 \\ V(r) \xrightarrow[r\to\infty]{} 0 \end{cases} \tag{51}$$

and $V(r) \in R + (L^\infty)_\epsilon$ which, in contrast with 'singular potentials' (Case 1950, Frank *et al* 1971), own a discrete lower-bounded spectrum. This analytic approach seems well suited for the study of the $gr^{-(s+2)}$ potential; the general matrix element of the operator replacing the Schrödinger operator is a very simple function of the exponent s and the angular momentum l. Let us also mention that in addition to the spectrum of energy levels the wavefunctions can easily be tabulated (Gazeau and Maquet 1979).

These results can immediately be extended to non-integer values of the angular momentum $l (l > -1/2)$ (replacing the factorial functions by a gamma function in the expression of the matrix elements $\Lambda_{ij}(s, l)$). This is therefore applicable to the study of confining potentials of the r^β kind ($\beta > 0$). Indeed, the following transformation of the dependent and independent variables,

$$r' = r^{-s/2}, \qquad \chi(r') = r^{-(s+2)/4}\eta(r), \tag{52}$$

($\eta(r) = R(r)r$ where $R(r)$ is the radial part of the wavefunction) changes the potential $-gr^{-(s+2)}$ with energy levels $E_q(s, l)$ into a potential $g'r'^\beta$ [$g' > 0$, $\beta = -2(s+2)/s$] with energy levels $E'_q(\beta, l')$ where

$$l + \frac{1}{2} = \frac{2}{2+\beta}\left(l' + \frac{1}{2}\right), \qquad E'_q(\beta, l) = 4\left(\frac{\hbar^2}{2m}\right)^{(s+2)/2} \frac{(g's^2)^{-s/2}}{s^2 \lambda_q(s, l)} \tag{53}$$

Particular cases of these transformations have already been used by Rowley (1979) and Schwartz (1976).

Let us note that the numerical difficulties encountered for s close to zero appear for large values of β, while the problem is easy to solve for small values of β (just like for $-2 < s < -0{\cdot}5$).

Let us finally mention that by the transformation (51), the crossings of levels of different angular momenta l are related to the crossings of levels for confining potentials as indicated by Grosse and Martin (1978).

References

Baumgartner B 1979 *J. Phys. A: Math Gen.* **12** 459
Bethe H A and Salpeter E E 1957 *Handbuch der Physik* **V** 35 (Berlin: Springer)
Brezinski C 1977 *Lecture Notes in Mathematics* No 584 (Berlin: Springer)
Case K M 1950 *Phys. Rev.* **80** 797
Decarreau A, Dumont-Lepage M-Cl, Maroni P, Robert A and Ronveaux A 1978 *Ann. Soc. Sci. Bruxelles* T **92** I–II pp 57–81
Frank W M, David J L and Spector R M 1971 *Rev. Mod. Phys.* **43** 36
Gazeau J P 1978 *J. Math. Phys.* **19** 10141
—— 1979 *Lett. Math. Phys* **3** 285
Gazeau J P and Maquet A 1979 *Phys. Rev. A* **20** 727
Grosse H and Martin A 1978 *Nucl. Phys.* B. **132** 125
Landau L and Lifschitz E 1966 *Mécanique Quantique: Théorie non Relativiste* (Moscow: MIR)
Lemieux A and Bose A K 1969 *Ann. Inst. Henri Poincaré* **10** 259
Rowley N 1979 *J. Phys. A: Math Gen.* **12** L7
Schwartz C 1976 *J. Math. Phys.* **17** 863
Simon B 1971a *Commun. Math. Phys.* **21** 192
—— 1971b *Quantum Mechanics for Hamiltonians defined as Quadratic Forms* (Princeton: Princeton UP)
Sobolev S L 1938 *Mat. Sb* **46** 471
Wilf H S 1970 *Finite Sections of Some Classical Inequalities* (Berlin: Springer)