Green's operator for Hamiltonians with Coulomb plus polynomial potentials

2007 J. Phys. A: Math. Theor. 40 7721

(http://iopscience.iop.org/1751-8121/40/27/020)

J. Phys. A: Math. Theor. **40** (2007) 7721–7728 doi:10.1088/1751-8113/40/27/020

Green's operator for Hamiltonians with Coulomb plus polynomial potentials

E Kelbert, A Hyder, F Demir, Z T Hlousek and Z Papp

Department of Physics and Astronomy, California State University, Long Beach, CA 90840, USA

Received 27 December 2006, in final form 24 May 2007
Published 20 June 2007
Online at stacks.iop.org/JPhysA/40/7721

Abstract
The Hamiltonian of a Coulomb plus polynomial potential in the Coulomb–Sturmian basis has an infinite symmetric band-matrix structure. A band matrix can always be considered as a block-tridiagonal matrix. So, the corresponding Green's operator can be given as a matrix-valued continued fraction. As examples, we calculate Green's operator for the Coulomb plus linear and quadratic confinement potential problems and determine the energy levels.

PACS number: 03.65.Nk

1. Introduction

Coulomb plus polynomial potentials,

$$v(r) = \sum_{i=-1}^{k} a_i r^i = a_{-1}/r + a_0 + a_1 r + a_2 r^2 + \cdots, \tag{1}$$

are often used to model various physical phenomena. The Coulomb potential, $v(r) = a_{-1}/r$, describes the interaction between charged particles. A Coulomb plus linear potential, $v(r) = a_{-1}/r + a_1 r$, also known as the Cornell potential, is the most common potential for modelling the confining quark interaction. It is also used in atomic physics to describe the Stark effect which occurs when the hydrogen atom is placed in an electric field. The two-dimensional Coulomb plus quadratic potential, $v(r) = a_{-1}/r + a_2 r^2$, is related to the Zeeman effect; the hydrogen atom in a magnetic field. The quartic harmonic oscillator potential, $v(r) = a_2 r^2 + a_4 r^4$, is used in field theory to model the spontaneous breaking of symmetry. It is evident that there is a great deal of physics that depends on the precise knowledge of the dynamics of the Coulomb potential with various polynomial interactions.

Over the years, several approaches have been developed to study some special cases of this problem (for a recent review see [1]). To the best of our knowledge, no method has been proposed yet that could treat this problem with an arbitrary potential strength a_i and arbitrarily high power of k.

In this work, we calculate Green's function of the non-relativistic quantum Hamiltonian with a Coulomb plus polynomial potential. Green's function of polynomial potentials in the harmonic oscillator basis has been calculated before [2, 3]. The use of the Coulomb–Sturmian basis will allow us to incorporate the Coulomb potential.

If we know Green's operator, then we have a complete knowledge of the physical system. For example, the eigenvalues of the Hamiltonian coincide with the poles of Green's operator. The corresponding eigenvectors can be determined from the relation

$$|\psi_n\rangle\langle\psi_n| = \frac{1}{2\pi \mathrm{i}} \oint_C G(z)\,\mathrm{d}z, \tag{2}$$

where C encircles the eigenvalue E_n in a counterclockwise direction without incorporating other poles.

In our previous works [4, 5], the Coulomb Green's operator was calculated in the Coulomb–Sturmian basis. In this basis, the operator $J = z - H$ has an infinite symmetric tridiagonal, i.e. Jacobi or J-matrix structure, where z is a complex number. We have shown that Green's operator $G(z) = (z - H)^{-1} = J^{-1}$ can be calculated in terms of continued fractions. This Coulomb Green's operator was used to solve the Faddeev integral equations of the three-body Coulomb problem [6].

In the Coulomb–Sturmian basis, the Hamiltonian with potential (1) is represented by an infinite symmetric band matrix. An infinite band matrix can always be considered as a block-Jacobi matrix with $m \times m$ blocks, where m is finite. Thus, the continued fraction becomes a matrix-valued continued fraction.

This paper is organized as follows. In section 2, we introduce the D-dimensional Coulomb–Sturmian basis. In section 3, we calculate the infinite band matrix representation of the Hamiltonian. In section 4, we derive the matrix continued fraction for Green's operator. Some applications are considered in section 5. First, to demonstrate the power of the method we show an analytically known case, the harmonic oscillator in two and three dimensions. Then we consider the Coulomb plus linear confinement potential, $v(r) = a_{-1}/r + a_1 r$, in three dimensions and the Coulomb plus quadratic confinement potential, $v(r) = a_{-1}/r + a_2 r^2$, in two dimensions.

2. The Coulomb–Sturmian basis

The kinetic energy operator in D dimension, with $D \geqslant 2$, is given by

$$H_0 = -\frac{1}{2}\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{L(L+1)}{r^2}\right), \tag{3}$$

where $L = l + (D-3)/2$. The Coulomb–Sturmian (CS) functions are the solutions of the Sturm–Liuoville problem of the Coulomb Hamiltonian [7]

$$\left(H_0 - \frac{\lambda}{r}\right)\langle r|n\rangle = -\frac{b^2}{2}\langle r|n\rangle, \tag{4}$$

where $b > 0$ is a parameter, n is the radial quantum number, $n = 0, 1, \ldots,$ and $\lambda = (n + L + 1)b$. In coordinate space, the CS functions are given by

$$\langle r|n\rangle = \left[\frac{\Gamma(n+1)}{\Gamma(n+2L+2)}\right]^{1/2} \mathrm{e}^{-br}(2br)^{L+1} L_n^{2L+1}(2br), \tag{5}$$

where L_n^{α} is an associated Laguerre polynomial. The CS functions form a basis. With $\langle r|\tilde{n}\rangle = 1/r\langle r|n\rangle$, we have the orthogonality

$$\langle\tilde{n}|n'\rangle = \langle n|\tilde{n}'\rangle = \langle n|1/r|n'\rangle = \delta_{nn'}, \tag{6}$$

and the completeness relations

$$\sum_{n=0} |n\rangle\langle\tilde{n}| = \sum_{n=0} |\tilde{n}\rangle\langle n| = \mathbf{1}. \tag{7}$$

3. Band-matrix representation

We consider the Hamiltonian

$$H = H_0 + \sum_{i=-1}^{k} a_i r^i \tag{8}$$

on the CS basis.

By utilizing the relations

$$L_n^\alpha = L_n^{\alpha+1} - L_{n-1}^{\alpha+1} \tag{9}$$

and

$$\int_0^\infty \exp(-x) x^\alpha L_n^\alpha(x) L_{n'}^\alpha(x)\,\mathrm{d}x = \frac{\Gamma(n+\alpha+1)}{\Gamma(n+1)}\delta_{n,n'}, \tag{10}$$

we can easily calculate the overlap of the CS states

$$\langle n|n'\rangle = \langle n'|n\rangle = \begin{cases} \dfrac{1}{b}(n+L+1) & \text{for} \quad n = n', \\ -\dfrac{1}{2b}\sqrt{n'(n'+2L+1)} & \text{for} \quad n' = n+1, \\ 0 & \text{for} \quad n' > n+1. \end{cases} \tag{11}$$

Then starting from equation (4), and using equations (6) and (11), we can derive the CS matrix elements of the kinetic energy operator

$$\langle n|H_0|n'\rangle = \langle n'|H_0|n\rangle = \begin{cases} \dfrac{b}{2}(n+L+1) & \text{for} \quad n' = n, \\ \dfrac{b}{4}\sqrt{n'(n'+2L+1)} & \text{for} \quad n' = n+1, \\ 0 & \text{for} \quad n' > n+1. \end{cases} \tag{12}$$

From equations (6), (11) and (12), it follows that the Hamiltonian $H = H_0 + a_{-1}/r + a_0$ is tridiagonal on the CS basis.

By further utilizing equations (9) and (10), we can also derive the following matrix elements

$$\langle n|r|n'\rangle = \langle n'|r|n\rangle = \begin{cases} \dfrac{1}{4b^2}(6n^2 + 2(L+1)(6n+2L+3)) & \text{for} \quad n' = n, \\ -\dfrac{1}{2b^2}(2n'+2L+1)\sqrt{n'(n'+2L+1)} & \text{for} \quad n' = n+1, \\ \dfrac{1}{4b^2}\sqrt{n'(n'-1)(n'+2L)(n'+2L+1)} & \text{for} \quad n' = n+2, \\ 0 & \text{for} \quad n' > n+2, \end{cases} \tag{13}$$

and

$$\langle n|r^2|n'\rangle = \langle n'|r^2|n\rangle$$
$$= \begin{cases} \frac{1}{8b^3}[(((10n+2L+4)(n+2L+3)+9n(n-1))(n+2L+2)+n(n-1)(n-2))] & \text{for} \quad n'=n, \\ -\frac{3}{8b^3}[(4n'+2L)(n'+2L+2)+(n'-1)(n'-2)]\sqrt{n'(n'+2L+1)} & \text{for} \quad n'=n+1, \\ \frac{3}{8b^3}(2n'+2L)\sqrt{n'(n'-1)(n'+2L+1)(n'+2L)} & \text{for} \quad n'=n+2, \\ -\frac{1}{8b^3}\sqrt{n'(n'-1)(n'-2)(n'+2L+1)(n'+2L)(n'+2L-1)} & \text{for} \quad n'=n+3, \\ 0 & \text{for} \quad n'>n+3. \end{cases} \tag{14}$$

Similarly, one can derive $\langle n|r^k|n'\rangle$ CS matrix elements for $k > 2$ as well. If k is finite, the Hamiltonian is an infinite symmetric band matrix, if $k = 1$, it is a pentadiagonal, and if $k = 2$, it is a septadiagonal band matrix.

4. Matrix continued fraction representation of Green's operator

Green's operator G is formally defined by the equation

$$J(z)G(z) = G(z)J(z) = 1, \tag{15}$$

where $J(z) = z - H$ and z is a complex number. On the CS basis, this takes the form

$$\sum_{i'} \langle i|J(z)|i'\rangle\langle\tilde{i'}|G(z)|\tilde{i''}\rangle = \delta_{i,i''}. \tag{16}$$

Now the operator $J(z)$ has an infinite symmetric band-matrix structure. An infinite symmetric band matrix can always be considered as a block-tridiagonal or a block-Jacobi matrix. So, equation (16) looks like

$$\begin{pmatrix} J_{0,0} & J_{0,1} & 0 & 0 & \cdots \\ J_{1,0} & J_{1,1} & J_{12} & 0 & \cdots \\ 0 & J_{2,1} & J_{2,2} & J_{2,3} & \cdots \\ 0 & 0 & J_{3,2} & J_{3,3} & \cdots \\ \vdots & \ddots & \ddots & \ddots & \ddots \end{pmatrix} \times \begin{pmatrix} G_{0,0} & G_{0,1} & G_{0,2} & G_{0,3} & \cdots \\ G_{1,0} & G_{1,1} & G_{1,2} & G_{1,3} & \cdots \\ G_{2,0} & G_{2,1} & G_{2,2} & G_{2,3} & \cdots \\ G_{3,0} & G_{3,1} & G_{3,2} & G_{3,3} & \cdots \\ \vdots & \ddots & \ddots & \ddots & \ddots \end{pmatrix}$$
$$= \begin{pmatrix} 1 & 0 & 0 & 0 & \cdots \\ 0 & 1 & 0 & 0 & \cdots \\ 0 & 0 & 1 & 0 & \cdots \\ 0 & 0 & 0 & 1 & \cdots \\ \vdots & \ddots & \ddots & \ddots & \ddots \end{pmatrix}, \tag{17}$$

where $J_{n,n'}$ and $G_{n,n'}$ are $m \times m$ block matrices, and the 1's and 0's are $m \times m$ unit and null matrices, respectively.

Just knowing the $N \times N$ upper-left corner of the full Green's matrix is sufficient to determine physical quantities. Let us denote the corresponding $N \times N$ upper-left corner block matrices by $J^{(N)}$, $G^{(N)}$ and $1^{(N)}$, respectively. If we multiply the $N \times \infty$ part of J with the $\infty \times N$ part of G, then we get the $N \times N$ block unit matrix $1^{(N)}$. The sum, due to the block tridiagonal form of J, is reduced to three block terms

$$J_{n,n-1}G_{n-1,n'} + J_{n,n}G_{n,n'} + J_{n,n+1}G_{n+1,n'} = \delta_{n,n'}, \tag{18}$$

where $n = 0, 1, \ldots, N$ and $n' = 0, 1, \ldots, N$. If $n < N$, only the terms from $G^{(N)}$ are participating in the sum. For $n = N$, an extra block matrix $G_{N+1,n'}$ outside the truncated subspace is needed:

$$J_{N,N-1}G_{N-1,n'} + J_{N,N}G_{N,n'} + J_{N,N+1}G_{N+1,n'} = \delta_{N,n'}. \tag{19}$$

We can formally eliminate this block by writing

$$J_{N,N-1}G_{N-1,n'} + [J_{N,N} + J_{N,N+1}G_{N+1,n'}(G_{N,n'})^{-1}]G_{N,n'} = \delta_{N,m}. \tag{20}$$

This formal elimination of the elements outside of $G^{(N)}$ amounts to modifying the $J_{N,N}$ block of $J^{(N)}$.

We can calculate $G_{N+1,n'}(G_{N,n'})^{-1}$ from another relation:

$$J_{N+1,N}G_{N,n'} + J_{N+1,N+1}G_{N+1,n'} + J_{N+1,N+2}G_{N+2,n'} = 0. \tag{21}$$

By introducing the notation

$$C_{N+1} = -G_{N+1,n'}(G_{N,n'})^{-1}(J_{N+1,N})^{-1}, \tag{22}$$

equation (21) can be rearranged as

$$C_{N+1} = (J_{N+1,N+1} - J_{N+1,N+2}C_{N+2}J_{N+2,N+1})^{-1}. \tag{23}$$

A repeated application of this relation results in a continued fraction with block matrices

$$C_{N+1} = (J_{N+1,N+1} - J_{N+1,N+2}(J_{N+2,N+2} - J_{N+2,N+3}(J_{N+3,N+3} - \cdots)^{-1}J_{N+3,N+2})^{-1}J_{N+2,N+1})^{-1}. \tag{24}$$

This matrix continued fraction does not depend on the index n' and the correction term to $J_{N,N}$ is the same for all n'. Therefore, we can write equation (20) in the form

$$\left(J^{(N)}_{i,j} - \delta_{i,N}\delta_{j,N}J_{N,N+1}C_{N+1}J_{N+1,N}\right)G^{(N)} = 1^{(N)}, \tag{25}$$

i.e. the modified $N \times N$ block-Jacobi matrix is the inverse of $G^{(N)}$:

$$(G^{(N)})^{-1} = J^{(N)}_{i,j} - \delta_{i,N}\delta_{j,N}J_{N,N+1}C_{N+1}J_{N+1,N}. \tag{26}$$

The numerical evaluation of matrix continued fractions is very similar to those of ordinary continued fractions. In backward evaluation we start at some $K > N$ term, neglect the higher terms, and evaluate (24) from the inside out. If a new approximant with larger K is needed, we have to start the whole process again. On the other hand, the backward evaluation is simple and provides very accurate results.

5. Examples

To demonstrate the power of this method, we take first the harmonic oscillator

$$H = H_0 + 1/2\omega^2 r^2 \tag{27}$$

in two and three dimensions. This Hamiltonian has a septadiagonal structure on the CS basis, which can be considered as a block-Jacobi matrix with 3×3 blocks. In our numerical example, we take $\omega = 1$ and roll up the continued fraction up to the first block and calculate the determinant of a 3×3 matrix. Figure 1 shows the poles of $G^0(z)$ as a function of the CS parameter b. We took $l = 0$, which implies $L = 0$ for $D = 3$ and $L = -1/2$ for $D = 2$, respectively. It can be seen that even a 3×3 Green's matrix provides all the eigenvalues

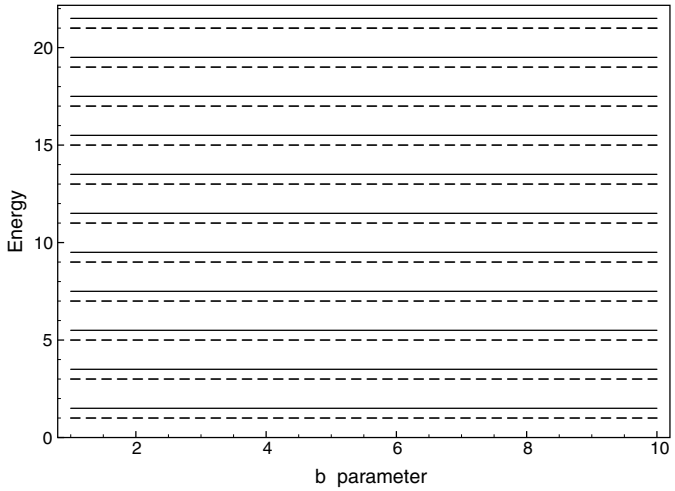

Figure 1. Eigenvalues of the three-dimensional (full line) and the two-dimensional (broken line) harmonic oscillator as a function of the CS basis parameter b.

of (27). They agree with the exact results $E_n = \omega(2n + L + 3/2)$ up to machine accuracy and the results are independent of the choice for the parameter b of the CS basis.

By using (2) we can also calculate the wavefunction ψ_n. From the contour integral of Green's matrix around E_n,

$$\langle \tilde{i}|\psi_n\rangle\langle\psi_n|\tilde{i}'\rangle = \frac{1}{2\pi \mathrm{i}} \oint_C \langle \tilde{i}|G(z)|\tilde{i}'\rangle \, \mathrm{d}z, \tag{28}$$

we can extract the overlap $\langle \tilde{i}|\psi_n\rangle$. If we take a small radius, about $r_0 = 0.1$, then we need about 20–30 Gauss–Legendre points to achieve machine accuracy. For the overlap of the harmonic oscillator and the CS functions, we got perfect agreements with the exact Maple results.

Next, we consider the Coulomb plus linear potential in three dimensions:

$$H = H_0 + Z/r + \alpha r, \tag{29}$$

and the Coulomb plus quadratic potential in two dimensions:

$$H = H_0 + Z/r + 1/2\omega^2 r^2. \tag{30}$$

The Hamiltonian (29) is pentadiagonal, and can be considered as a block-Jacobi matrix with 2×2 blocks, while (30) is septadiagonal, like in the harmonic oscillator case. For the numerical values we take $Z = -1, \alpha = 1$ and $\omega = 1$. The lowest 20 eigenvalues are given in table 1. We observed a similar stability with respect to varying b as we did in the case of the harmonic oscillator. This we can expect because these cases, on the CS basis, are not more complicated than the harmonic oscillator problem.

We also tried the Coulomb plus linear confinement with the negative α, which is relevant in the Stark effect. In this case, the continued fraction fails to converge. This situation reminds us of the problem we had with the Coulomb Green's operator at positive energy, when the continued fraction also failed to converge. The solution was the analytic continuation of continued fractions [5]. It seems that we need to find an analogous procedure for matrix continued fractions.

Table 1. Eigenvalues of Hamiltonians with the Coulomb plus linear potential in three dimensions and the Coulomb plus quadratic potential in two dimensions. The potential parameters are $Z = -1, \alpha = 1$ and $\omega = 1$.

n	Equation (29)	Equation (30)
1	0.577 921 351 961	−1.836 207 439 051
2	2.450 162 895 052	1.576 895 542 024
3	3.756 905 691 262	3.828 388 290 161
4	4.855 671 243 373	5.963 137 645 126
5	5.836 029 886 654	8.052 626 115 348
6	6.736 620 996 511	10.118 396 975 26
7	7.578 378 030 294	12.169 728 962 61
8	8.374 205 689 360	14.211 427 220 55
9	9.132 754 730 978	16.246 284 530 60
10	9.860 176 266 906	18.276 058 941 34
11	10.561 039 609 14	20.301 924 139 05
12	11.238 855 637 15	22.324 699 927 91
13	11.896 395 442 11	24.344 979 875 08
14	12.535 894 616 58	26.363 206 506 47
15	13.159 189 823 53	28.379 717 862 76
16	13.767 813 305 61	30.394 777 528 67
17	14.363 060 217 27	32.408 594 679 47
18	14.946 037 799 01	34.421 337 860 62
19	15.517 702 067 15	36.433 144 701 88
20	16.078 885 704 44	38.444 128 917 67

6. Summary and conclusions

In this work, we have shown that in the D-dimensional Coulomb–Sturmian basis the non-relativistic D-dimensional Hamiltonian with the Coulomb plus polynomial potential has a band-matrix structure. A band matrix can always be considered as a block-Jacobi matrix, and, consequently, Green's matrix can be constructed in terms of matrix continued fractions. A numerically converged matrix continued fraction gives a numerically exact Green's operator, which even on a very small basis provides the exact spectrum. We have demonstrated the power of the method in the case of a harmonic oscillator and obtained the exact spectrum. As examples, we studied the Coulomb plus linear confinement in three dimensions and the Coulomb plus quadratic confinement in two dimensions. The first one is related to the quark confinement, while the second one to the Zeeman effect. The exact knowledge of these Green's operators may facilitate the use of integral equations to describe quantum processes with constrained asymptotics.

Acknowledgment

This work has been supported by the Research Corporation.

References

[1] Plante G and Antippa A F 2005 *J. Math. Phys.* **46** 062108
[2] Graffi S and Grecchi V 1975 *Lett. Nuovo Cimento* **12** 425
[3] Znojil M and Majling L 1983 *J. Phys. A: Math. Gen.* **16** 639

[4] Demir F, Hlousek Z T and Papp Z 2006 *Phys. Rev.* A **74** 014701
[5] Kónya B, Lévai G and Papp Z 1997 *J. Math. Phys.* **38** 4832
[6] See, e.g., Papp Z 1997 *Phys. Rev.* C **55** 1080
Papp Z, Hu C-Y, Hlousek Z T, Kónya B and Yakovlev S L 2001 *Phys. Rev.* A **63** 062721
Papp Z, Darai J, Mezei J Zs, Hlousek Z T and Hu C-Y 2005 *Phys. Rev. Lett.* **94** 143201
[7] Rotenberg M 1970 *Adv. At. Mol. Phys.* **6** 233