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Potential $r^2 + \lambda r^2/(1 + gr^2)$ and the analytic continued fractions

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Abstract. We construct the exact wavefunctions and an analytic (continued-fractional) Green function for the one- and three-dimensional Schrödinger equation with the potential

$$V(r) = h/r^2 + r^2 + \lambda r^2/(1 + gr^2), \quad h > -\frac{1}{4}; \lambda, g > 0.$$

In the numerical application of the formulae, the energy and norm of the bound state ψ may be approximated by both their lower and upper estimates.

1. Introduction

The Schrödinger equation with the simplest non-polynomial interaction added to the harmonic-oscillator Hamiltonian H_0

$$[H_0 + \lambda r^2/(1 + gr^2)]\psi(r) = \tilde{E}\psi(r), \quad \lambda > 0, g > 0, \quad (1)$$

finds applications in various branches of physics (quantum mechanics, field theory in zero dimensions, laser theory etc—see Biswas *et al* (1973) or Whitehead *et al* (1982) for references). It has been thoroughly studied by perturbative or variational methods (Mittra 1978, Kaushal 1979, Bessis and Bessis 1980) and the resulting efficient algorithms for its numerical solution are available. In the present note, inspired by a puzzling existence of one exact solution of (1) which has an elementary form (Flessas 1981, Varma 1981, Whitehead *et al* 1982), we intend to complement these results and construct all the ψ 's and \tilde{E} 's by purely analytic means.

We shall not distinguish between the one- and three-dimensional interpretation of the 'unperturbed' problem

$$\begin{aligned} H_0|n\rangle &= \varepsilon_n|n\rangle, & H_0 &= -d^2/dr^2 + l(l+1)/r^2 + r^2, \\ \varepsilon_n &= 4n + 2l + 3, & n &= 0, 1, \dots, \end{aligned} \quad (2)$$

and assume that we have either $l = -1, 0$ and $r \in (-\infty, \infty)$, or $l = 0, 1, 2, \dots$, and $r \in (0, \infty)$, respectively. In the latter case, we may also admit non-integer l 's when we denote the angular momenta by $\mathcal{L} = 0, 1, \dots$ and introduce an additional force h/r^2 , $h > -\frac{1}{4}$, such that $l(l+1) = \mathcal{L}(\mathcal{L}+1) + h$ (cf Killingbeck and Galicia 1980).

We shall start by proceeding along the same lines as in Whitehead *et al* (1982) and represent the Schrödinger equation (1) as an infinite-matrix 'diagonalisation'. Its

consequent non-numerical treatment gives an exact form of ψ and converts the Schrödinger eigenvalue problem into an analytic test of convergence of $\|\psi\|$ (§ 2). In § 3, we transform the corresponding convergence criterion into a boundary-value condition for the nonlinear two-term recurrences and show that this represents an efficient numerical algorithm for the computation of the energies. Finally, we prove that the physical energies coincide exactly with the zeros of a simple analytic continued fraction (§ 4).

2. Schrödinger equation in the harmonic-oscillator basis

In the first step of our considerations we multiply (1) by $1 + gr^2$ from the left and employ the completeness of $|n\rangle$'s,

$$\sum_{n=\max(0,m-1)}^{m+1} \langle m|(1+gr^2)|n\rangle(\epsilon_n - E)\langle n|\psi\rangle = F\langle m|\psi\rangle, \tag{3}$$

$$E = \tilde{E} - F, \quad F = \lambda/g, \quad m = 0, 1, \dots$$

This is an infinite and homogeneous system of the linear equations to be satisfied by the projections $\langle n|\psi\rangle$. We may distinguish the following two cases.

(i) The physical eigenvalue $E = E^{(i)}$ does not coincide with any of the oscillator energies ϵ_n . Then, we may put $\langle k|\psi\rangle = z_k/(\epsilon_k - E)$, and our Schrödinger equation (1) or (3) acquires the form

$$Q(\infty) \begin{pmatrix} z_0 \\ z_1 \\ \dots \end{pmatrix} = 0, \quad Q(\infty) = \begin{pmatrix} a_0 & b_0 & 0 & \dots \\ b_0 & a_1 & b_1 & 0 & \dots \\ 0 & b_1 & a_2 & \dots \\ \dots & \dots & \dots & \dots \end{pmatrix} \tag{4}$$

$$a_k = 1 - \frac{F}{\epsilon_k - E} + \frac{g\epsilon_k}{2}, \quad b_k = g[(k+1)(k+l+\frac{3}{2})]^{1/2}, \quad k = 0, 1, \dots$$

where the infinite-dimensional matrix $Q(\infty)$ is symmetric and tridiagonal.

(ii) Whenever the physical eigenvalue $E^{(i)}$ coincides with some ϵ_{N_i} , we have to replace the N_i th row in (3) by mere definition,

$$\langle N_i|\psi\rangle = (b_{N_i-1}z_{N_i-1} + b_{N_i}z_{N_i+1})/F, \tag{5a}$$

while the rest of (3) becomes decoupled into a pair of finite- and infinite-dimensional problems,

$$Q(N_i - 1) \begin{pmatrix} z_0 \\ z_1 \\ \dots \\ z_{N_i-1} \end{pmatrix} = 0, \quad Q(n) = \begin{pmatrix} a_0 & b_0 & 0 & \dots & 0 \\ b_0 & a_1 & b_1 & \dots & \\ \dots & \dots & \dots & \dots & \\ 0 & \dots & b_{n-1} & & a_n \end{pmatrix} \tag{5b}$$

and

$$\begin{pmatrix} a_{N_i+1} & b_{N_i+1} & 0 & \dots \\ b_{N_i+1} & a_{N_i+2} & \dots & \\ \dots & \dots & \dots & \dots \end{pmatrix} \begin{pmatrix} z_{N_i+1} \\ z_{N_i+2} \\ \dots \end{pmatrix} = 0, \tag{5c}$$

respectively. Obviously, we have now the following two possibilities for constructing a non-trivial solution z :

(1) Provided that $\det Q(N_i - 1) = 0$, we may complement the non-trivial solution of (5b) by the zero z 's in (5c). The resulting ψ is an elementary function, as noticed first by Flessas (1981) and described in detail by Whitehead *et al* (1982).

(2) When $\det Q(N_i - 1) \neq 0$, we must put $z_0 = \dots = z_{N_i-1} = 0$. Then the structure of (5c) is equivalent to (4) and need not be considered separately in what follows.

In the form (4), our problem is similar to the standard diagonalisation, but it must be treated with due care since its energy dependence is non-standard. Moreover, the compact formula

$$\langle n | \psi \rangle = \frac{(-1)^n (\epsilon_0 - E) \langle 0 | \psi \rangle}{(\epsilon_n - E) b_0 b_1 \dots b_{n-1}} \det Q(n-1), \quad n = 1, 2, \dots, \quad (6)$$

gives formally the explicit solution $|\psi\rangle = \sum |n\rangle \langle n | \psi \rangle$ for each energy E and normalisation $\langle 0 | \psi \rangle$. The physical requirement concerning $\psi(r)$'s,

$$\|\psi\|^2 = \sum_{n=0}^{\infty} |\langle n | \psi \rangle|^2 = \sum_{n=0}^{\infty} \frac{z_n^2}{(\epsilon_n - E)^2} < \infty, \quad (7)$$

may still be met by z 's possessing an infinite norm. Our approach to the solution of (4) will therefore be based on a direct verification of convergence (7) by means of the Raabe criterion (e.g. Korn and Korn 1968)

$$\lim_{n \rightarrow \infty} n (|\langle n | \psi \rangle / \langle n + 1 | \psi \rangle|^2 - 1) > 1 \Rightarrow \|\psi\| < \infty$$

$$< 1 \Rightarrow \|\psi\| = \infty. \quad (8)$$

3. Schrödinger equation as recurrences

3.1. Auxiliary sequences

To simplify the determinantal form (6) of the convergence criterion (8), we decompose algebraically the three-diagonal matrix $Q(\infty)$ in (4) into the product of the three simpler matrices

$$Q(\infty) = \begin{pmatrix} 1 & u_0 & 0 & \dots \\ 0 & 1 & u_1 & 0 & \dots \\ \dots & & & & \dots \end{pmatrix} \times \begin{pmatrix} 1/f_0 & 0 & \dots \\ 0 & 1/f_1 & 0 & \dots \\ \dots & & & & \dots \end{pmatrix}$$

$$\times \begin{pmatrix} 1 & 0 & \dots \\ d_1 & 1 & 0 & \dots \\ 0 & d_2 & 1 & 0 & \dots \\ \dots & & & & \dots \end{pmatrix} \quad (9)$$

where $u_k = b_k f_{k-1}$, $d_k = b_{k-1} f_k$, and f_0, f_1, \dots is an arbitrary sequence which satisfies the recurrences

$$1/f_k = a_k - b_k^2 f_{k+1}, \quad k = 0, 1, \dots \quad (10)$$

Then equation (4) may also be decomposed,

$$\begin{pmatrix} 1 & & & \\ d_1 & 1 & & \\ & d_2 & 1 & \\ \dots & & & \dots \end{pmatrix} \begin{pmatrix} z_0 \\ z_1 \\ z_2 \\ \dots \end{pmatrix} = \begin{pmatrix} w_0 \\ w_1 \\ w_2 \\ \dots \end{pmatrix}, \quad \begin{pmatrix} 1 & u_0 & & \\ & 1 & u_1 & \\ & & \dots & \dots \end{pmatrix} \begin{pmatrix} 1/f_0 \\ & 1/f_1 & & \\ & & \dots & \dots \end{pmatrix} \begin{pmatrix} w_0 \\ w_1 \\ \dots \end{pmatrix} = 0, \quad (11)$$

and solved in a compact form

$$w_k = (-1)^k w_0 / t_0 t_1 \dots t_{k-1}, \quad w_0 = z_0, \quad t_{k-1} = b_{k-1} f_{k-1},$$

$$z_k = w_k - z_{k-1} d_k = (-1)^k \left[1/t_0 \dots t_{k-1} + \sum_{j=2}^k \left(\prod_{n=0}^{j-2} d_{k-n} \right) \right. \\ \left. \times \left(\prod_{m=0}^{k-j} t_m \right)^{-1} + d_1 d_2 \dots d_k \right] z_0, \quad k = 1, 2, \dots, \quad (12)$$

in terms of f 's. We may verify that (12) is equivalent to (6) and independent of the initialisation of the auxiliary sequence f_k . Nevertheless, the particular sequence $f_k^{(0)}$ denoted by the zero superscript and defined by the initialisation

$$1/f_0^{(0)} = 0 \quad (13)$$

gives by far the simplest form of z 's

$$z_k = (-1)^k z_0 b_0 f_1^{(0)} b_1 f_2^{(0)} \dots b_{k-1} f_k^{(0)}, \quad (14)$$

which is also especially suitable for an insertion into (8).

3.2. Determination of the eigenvalues

The $k \gg 1$ approximate form of (10) for $\varphi_k = gk f_k$,

$$1/\varphi_k = 2 - \varphi_{k+1} + O(1/k), \quad (15)$$

is an approximately k -independent mapping with a unique (semi-stable) point of accumulation. After a sufficient number of iterations, we obtain $\varphi_k \sim 1$ from any initialisation φ_N . This type of 'convergence' is quite quick—e.g. from $\varphi_N = 0$ we get $\varphi_{N-i} = i/(i+1) + O(1/N)$ for $i = 1, 2, \dots$.

The resulting rough estimate of $z_k/z_{k+1} = -1/b_k f_{k+1}^{(0)} = O(1)$ shows that the distinction between the convergent and divergent $\|\psi\|$'s has to be attributed to the higher-order corrections.

When we denote the first correction by $\Delta_k = gk f_k - 1$, we obtain the old recurrences (10) in the new $k \gg 1$ form

$$\Delta_k = \frac{\Delta_{k+1} - 1/gk + O(1/k^2)}{1 + (1 - g\omega)/gk - \Delta_{k+1}}, \quad \omega = l + \frac{3}{2}. \quad (16)$$

The mappings $\Delta_{k+1} \rightarrow \Delta_k$ or $\Delta_k \rightarrow \Delta_{k-1}$ are still only weakly k -dependent for $k \gg 1$. Their geometric interpretation is presented in figure 1 and shows that the sequence of Δ_k 's initialised by some Δ_N has now the two distinct (weakly k -dependent) points of accumulation

$$\Delta_k \sim \Delta_k^{(-)} = -(gk)^{-1/2} + O(1/k), \quad 1 \ll k \ll N, \quad (17a)$$

$$\Delta_k \sim \Delta_k^{(+)} = +(gk)^{-1/2} + O(1/k), \quad k \gg N. \quad (17b)$$

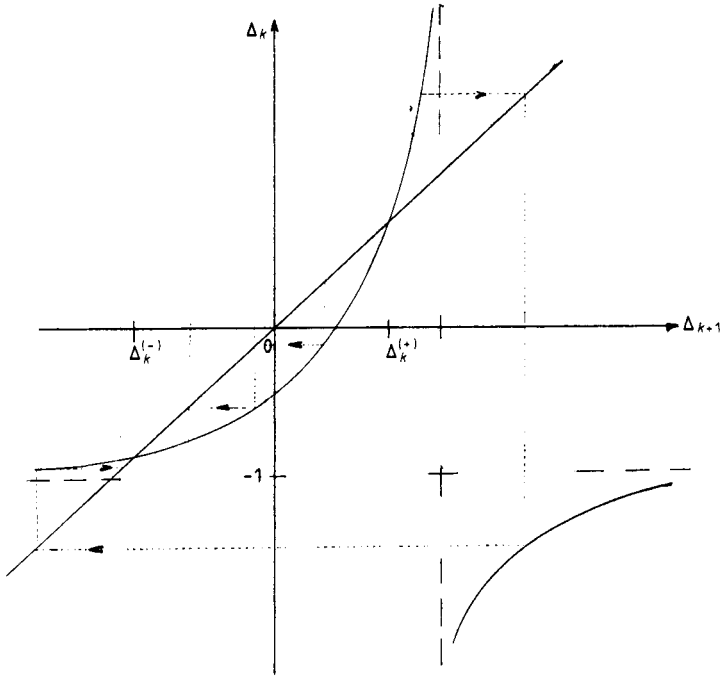


Figure 1. Geometric interpretation of the mapping $\Delta_{k+1} \rightarrow \Delta_k$.

In the light of equations (17), a set of all the possible sequences f_k interpreted as functions of $k \gg 1$ has the form depicted in figure 2. These non-intersecting curves may be reinterpreted also as the same particular sequence (say, $f_k^{(0)}$) at the different

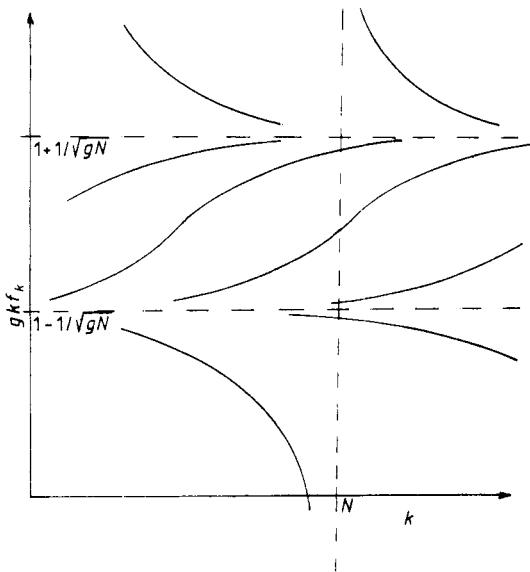


Figure 2. The $k \gg 1$ asymptotic behaviour of the different f_k .

energies E . For almost all E 's, we get therefore an asymptotic estimate (cf (13) and (17b))

$$z_k/z_{k-1} = -b_{k-1}f_k^{(0)} = -(1 + (gk)^{-1/2} + O(1/k)) \tag{18}$$

and an infinite norm of ψ (cf (8)). *Vice versa*, whenever $\|\psi\| < \infty$, the physical requirement $E = E^{(i)}$ may be given the form of the transcendental equation

$$b_{k-1}f_k^{(0)} = 1 - (gk)^{-1/2} + c(k)/k, \quad c(k) \neq 2(k/g)^{1/2}, \quad k = N_0 \gg 1, \tag{19}$$

reflecting the non-stability of the physical solution $f_k^{(0)}$ at $E = E^{(i)}$.

3.3. Numerical test

The recurrences (10) complemented by the ‘boundary conditions’ (13) and (19) with the finite and growing N_0 's represent a systematic sequence of approximations to the Schrödinger eigenvalue problem (1). The efficiency of this scheme has been verified numerically and a sample of the results is given in table 1. The three algorithms A1, A2 and A3 were used, with the respective initialisations (13), (19) and (19), and with the respective choice of $c(N_0) = 0$, $c(N_0) = 0$ and $c(N_0) \gg 2(N_0/g)^{1/2}$ in equation (19). The ‘exact’ energies of Bessis and Bessis (1980) were reproduced, or, for $\lambda = g = 1$, corrected in accordance with Mitra (1978). For small couplings, the convergence was found to be excellent—sometimes, even the $N = 2$ approximation gives fair results.

From the practical point of view, the most important property of the pair of algorithms A2 and A3 is that they generate the pair of the lower and upper bounds for the energies—this follows from figure 1 and informs us directly about the precision of the approximate result.

For the ‘subcritical’ N_0 's, even the unstable algorithm A1 gives satisfactory approximations. Of course, it must be used with great caution—e.g., the ground-state root of (19) disappears completely at $N_0 = 20$ for $\lambda = g = 0.1$.

4. Analytic solution

In the limit $N_0 \rightarrow \infty$, the discrete eigenvalue problem (10)+(13)+(19) becomes equivalent to (1)—we may prove our final analytic result.

Theorem. The physical energies $E = E^{(i)}$ coincide with the poles of an analytic continued fraction $f_0^{(\infty)}$ defined by (10).

Proof. By definition (Wall 1948) we have $f_k^{(\infty)} = \lim_{N \rightarrow \infty} f_k^{(N)}$, $k = 0, 1, \dots$, where $f_k^{(N)}$ is a particular auxiliary sequence f_k initialised by the value $1/f_N^{(N)} = 0$. Such a sequence is singular ($f_{N-1}^{(N)} = 0$, $f_N^{(N)} = \infty$, $f_{N+1}^{(N)} = a_N/b_N^2, \dots$) but it may still be used to define z 's since all the indefinite products and sums of the singular terms in (12) (namely, $f_{N-1}^{(N)}f_N^{(N)} = -1/b_N^2$ and $b_{N-1}f_N^{(N)} + 1/b_{N-1}f_{N-1}^{(N)} = a_{N-1}/b_{N-1}$, respectively) are finite. The convergence of the continued fractions $f_k^{(\infty)}$ follows from (17a) and implies that equation (19) is satisfied. It may be reinterpreted as a ‘coincidence’ condition $f_k^{(0)} = f_k^{(\infty)}$ valid for all k 's at $E = E^{(i)}$. From the same point of view, we may reinterpret equation (13) written in the form

$$1/f_k^{(\infty)} = 0 \tag{20}$$

as the standard secular equation for $E^{(i)}$'s.

Table 1. Binding energies—convergence of the deviations $d = (E_{\text{computed}} - E_{\text{exact}}) \times 10^9$.

$E_{\text{exact}} = 1.043\ 173\ 710^a$		$5.181\ 094\ 790^b$		
N_0	A2 ^c	A3 ^c	A2	A3
2	-30 804	+90 198	-4 531	+312 947
3	-1 242	+3 467	-61	+346
4	-70	+194	-4	+12
5	-2	+16	-0.4	+0.9
6	+2	+3	-0.04	+0.07
7	+2	+2	-0.008	+0.006

$E_{\text{exact}} = 1.000\ 841\ 100^d$		$9.976\ 180\ 090^e$			
N_0	A2	A3	N_0	A2	A3
200	-603	+109	50	-444	+308
300	-111	+30	100	-2	-2

$E_{\text{exact}} = 1.043\ 173\ 710^a$		$1.836\ 385\ 000^g$	
N_0	A1 ^c	N_0	A1
3	-89	90	+965
5	-0.011	110	-643
6	-0.003	130	-713
7	-0.010	150	-529
12	-228	250	-60
15	-39 783		

$E_{\text{exact}} = 1.232\ 372\ 050^f$		$1.836\ 385\ 000^g$			
N_0	A2	A3	N_0	A2	A3
11	-31 219	+8 177	300	-129 612	+29 922
12	-23 202	-1 404	400	-38 995	+7 348
13	-18 907	-6 552	500	-16 158	+175
20	-13 466	-13 085	600	-8 941	-2 454

^a $\lambda = g = 0.1$, ground state.
^b $\lambda = g = 0.1$, second excited state.
^c Algorithms described in § 3.3.
^d $\lambda = 0.1$, $g = 100$, ground state.
^e $\lambda = 100$, $g = 0.1$, ground state.
^f $\lambda = g = 1$, ground state (see the comment in § 3.3).
^g $\lambda = g = 100$, ground state.

A slight modification of this result confirms the applicability of the standard truncation method to equation (4).

Corollary 1. The finite secular equation

$$\det Q(N) = 0, \quad N < \infty, \tag{21}$$

gives the approximate roots $E = E^{(i)}(N)$ which converge towards the exact physical energies $E^{(i)}$ in the limit $N \rightarrow \infty$.

Proof. From $1/f_{k+1}^{(N+2)} = 0$ it follows that $1/f_k^{(N+2)} f_{k+1}^{(N+2)} \neq 0$ (cf the proof of theorem). Hence, the algebraic identity

$$\det Q(N) = 1/f_0^{(N+2)} f_1^{(N+2)} \dots f_N^{(N+2)} \tag{22}$$

implies that the roots $E^{(i)}(N)$ of the finite determinant $\det Q(N)$ coincide with the roots of the finite approximants $1/f_0^{(N+2)}$ to equation (20) and *vice versa*.

We may introduce here also the so-called effective interactions.

Corollary 2. The finite secular equation

$$\det Q^{(M)}(N) = 0, \quad N < \infty, \quad M \leq \infty \tag{23}$$

with the ‘effective Hamiltonian’ matrix

$$Q^{(M)}(N)_{ij} = Q(N)_{ij} - \delta_{iN}\delta_{jN}b_N^2 \frac{f_N^{(N+M+2)}}{f_{N+1}^{(N+M+2)}}, \quad i, j = 0, 1, \dots, N, \tag{24}$$

gives the energies $E^{(i)}(N+M)$ which become exact in the limit $M \rightarrow \infty$.

Proof. In accord with (22) and (10), the replacement of the matrix element $a_N \rightarrow a_N^{(M)} = 1/f_N^{(N+M+2)}$ in (21) is equivalent to the replacement of the cut-off $N \rightarrow N+M$ since the initialisation $f_{N+1}^{(N+2)} = 0$ of our auxiliary sequence $f_k^{(N+2)(M)}$ may be given an equivalent form $1/f_N^{(N+2)(M)} = a_N^{(M)} = 1/f_N^{(N+M+2)}$.

For practical purposes, we may employ either the $M \rightarrow \infty$ limit or the various approximate forms of (24).

Corollary 3. The finite secular equation (23) with $N \gg 1$ may be replaced by

$$\det Q_{(c)}(N) = 0 \tag{25}$$

$$Q_{(c)}(N)_{ij} = Q(N)_{ij} - \delta_{iN}\delta_{jN}b_N(1 - (gN)^{-1/2} + c/N), \quad i, j = 0, 1, \dots, N,$$

with an arbitrary real constant c not lying in the $O(1/N)$ vicinity of $c(N) = 2(N/g)^{1/2}$. It improves the precision of equation (21) provided that $c = O(1)$. With the pair of constants $c = c_1 \in (0, c(N))$ and $c = c_2 \notin (0, c(N))$, we obtain the pairs of energy roots which approach the exact $E^{(i)}$ ’s from both sides in the limit $N \rightarrow \infty$.

Proof. With respect to the accumulation property (17a), the first part of our assertion follows from (23) with some $M \gg 1$ and with $b_N f_{N+1}^{(N+M+2)}$ in (24) replaced by an estimate (19). The second statement was inspired by the results of table 1 and follows from the smooth character of the E dependence of f_k ’s near $E^{(i)}$. It becomes obvious after an inspection of figure 1 or 2.

5. Conclusions

We would like to underline the following four aspects of the present formalism.

(1) In analogy with the results obtained recently for certain polynomial potentials by Singh *et al* (1978, 1979), our ‘Green function’ $f_0^{(\infty)}$ is a sum of its various perturbation expansions and exhibits their analytic properties in an explicit way. For certain exceptional energy and couplings specified by Whitehead *et al* (1982), it may also degenerate to the elementary (rational) function.

(2) The bound states are exactly defined by means of the closed formula (6). Up to the degenerate terminating solutions, they have a form of a convergent infinite-series expansion in the basis $|n\rangle$.

(3) From the numerical point of view, formula (14) with $f_k^{(0)} = f_k^{(\infty)}$ gives an alternative and numerically stable prescription how to evaluate the determinantal bound-state projections $\langle n|\psi\rangle$ and the norm of ψ simultaneously with the generation of the inverse 'Green function' $1/f_0^{(\infty)}$ near or at its zero. It is important to keep in mind that the modified initialisations (cf algorithms A2 and A3) enable us to construct the lower and upper bounds for both the energy $E^{(i)}$ and norm $\|\psi\|$.

(4) In a broader context, our example and construction exhibit a close structural connection between the exact (continued-fractional) 'effective Hamiltonian' $Q^{(\infty)}(N)$ and the exact (continued-fractional) 'inverse Green function' $1/f_0^{(\infty)} = Q^{(\infty)}(0)$ (cf also Znojil 1980).

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Note added. An interesting paper by C S Lai and H E Lin (1982 *J. Phys. A: Math. Gen.* **15** 1495) appeared immediately after our submission. It describes another approach to the present problem and should be added to the list of references.

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