Bound and resonant states in Coulomb-like potentials

Bound and resonant states in Coulomb-like potentials

Z Papp

Institute of Nuclear Research of the Hungarian Academy of Sciences, H-4001 Debrecen, PO Box 51, Hungary

Abstract. The potential separable expansion method has been generalised to calculating bound and resonant states in Coulomb-like potentials. The complete set of Coulomb-Sturmian functions was taken as the basis to expand the short-range potential. On this basis the matrix elements of the Coulomb-Green functions have been given in closed form as functions of the (complex) energy. The feasibility of the method is demonstrated by a numerical example.

1. Introduction

In this paper we generalise a powerful approximation method, the potential separable expansion (PSE) method for calculating bound and resonant states in Coulomb-like potentials. The method was introduced by Révai (1975) and was rigorously founded by Gyarmati *et al* (1979). In these papers the advantages of the method compared with the other procedures were demonstrated and the relations to other methods were also cleared up. The PSE method was subsequently applied to various physical problems, namely to calculation of the bound states in short-ranged spherical (Révai 1975, Gyarmati *et al* 1979) and deformed (Gyarmati and Kruppa 1982) potentials, to the problem of two particles moving in a potential (Gareev *et al* 1979), to the quantum mechanical two-centre problem (Gareev *et al* 1977), to the binding energy of triton (Truhlik 1978) and was generalised to resonant (Gamow) (Gyarmati *et al* 1984, Kruppa and Papp 1985) and scattering states (Révai *et al* 1985). The method was also applied to calculating bound and resonant states in the framework of the orthogonality condition model (Pál 1985).

The philosophy underlying the method is the following. We split the Hamiltonian H into two parts, $H = H^0 + H'$, where H^0 is responsible for the asymptotic behaviour of the system and H' is the short-range interaction. The bound and Gamow states are the solution of the homogeneous Lippmann-Schwinger equation

$$|\psi\rangle = G^0(E)H'|\psi\rangle \tag{1.1}$$

belonging to the real and complex eigenvalues, respectively, where $G^0(E) = [E - H^0]^{-1}$ is the Green operator of H^0. The PSE method takes the interaction H' as a sum of separable terms

$$H' \approx \sum_{i,j=0}^{N} |i\rangle\langle i|H'|j\rangle\langle j| \tag{1.2}$$

where $\{|i\rangle\}$ is an orthonormal basis. So, instead of solving (1.1), we solve the equation

$$|\psi^N\rangle = G^0(E) \sum_{i,j=0}^{N} |i\rangle\langle i|H'|j\rangle\langle j|\psi^N\rangle \tag{1.3}$$

and the solutions of (1.1) are approximated by the solutions of (1.3), where N is an appropriate finite number. Equation (1.3) can be reduced to a system of homogeneous algebraic equations

$$\sum_{j=0}^{N} \left\{ \delta_{kj} - \sum_{i=0}^{N} \langle k|G^0(E)|i\rangle\langle i|H'|j\rangle \right\} C_j^N = 0 \qquad k = 0, 1, \ldots, N \tag{1.4}$$

where $C_j^N = \langle j|\psi^N\rangle$. Equation (1.4) is solvable if and only if

$$D(E) = \det\left\{ \delta_{kj} - \sum_{i=0}^{N} \langle k|G^0(E)|i\rangle\langle i|H'|j\rangle \right\} = 0. \tag{1.5}$$

$D(E)$ is just the Fredholm determinant of (1.3) and its zeros give the eigenvalues E_α^N. The index α stands for the quantum numbers of the states. According to (1.3), in the PSE method the wavefunction belonging to the eigenvalue E_α^N appears as

$$|\psi_\alpha^N\rangle = \sum_{i=0}^{N} b_{\alpha i}^N G^0(E_\alpha^N)|i\rangle \tag{1.6}$$

where $b_{\alpha_i}^N = \Sigma_{j=0}^N \langle i|H'|j\rangle C_{\alpha j}^N$. Since the coefficients $C_{\alpha j}^N$ are determined uniquely within a factor, the coefficients $b_{\alpha i}^N$ can be fixed by the normalisation of the wavefunction

$$1 = \langle \psi_\alpha^N|\psi_\alpha^N\rangle = \sum_{i,j=0}^{N} b_{\alpha i}^{N*} b_{\alpha j}^N \langle i|G^{02}(E_\alpha^N)|j\rangle. \tag{1.7}$$

In the PSE method only the asymptotically irrelevant short-range potential is approximated, so if the calculation of the matrix elements $\langle i|G^0|j\rangle$ and the vectors $G^0|i\rangle$ do not contain approximations and the exact energy is well approximated, the wavefunction has the correct asymptotic behaviour. This advantage is especially striking in comparison with the method based on the expansion of the wavefunction (WFE) on a basis. In the WFE method the total Hamiltonian is truncated and the asymptotics of the wavefunction is determined by the asymptotics of the basis functions.

The various applications proved that the PSE method is an efficient approximation method. It is especially useful when the asymptotic part of the wavefunction plays an important role. In the previous applications the whole interaction was short-range type, i.e. the H^0 was just the kinetic energy operator H_0 and G^0 was the free Green operator G_0. The harmonic oscillator (HO) wavefunctions were used as a basis and the matrix elements of the operators G_0 and G_0^2 and the vectors $G_0|i\rangle$ were given in closed forms.

The Gamow states are not normalisable in the conventional sense, so they do not belong to the Hilbert space (Berggren 1968). The handling of Gamow states requires the use of a generalised inner product: the Gamow vector in bra position is to be substituted by its adjoint. In evaluating the generalised inner products needed for the PSE method we analytically continued the integrals from the physical energy sheet to the complex zero of $D(E)$ on the unphysical sheet (Kruppa and Papp 1985).

The aim of this paper is to generalise the method in another direction, namely to the case of the long-range Coulomb-like interactions. A Coulomb-like potential V can be written in the form

$$V = V_c + V_s \tag{1.8}$$

where $V_c = Z_1 Z_2 e^2 / r$ is the pure Coulomb potential and V_s is a short-range potential. In this case the asymptotic motion is determined by the kinetic energy and the potential V_c, so the bound and resonant states developing in the Coulomb-like potentials are solutions to the homogeneous Lippmann–Schwinger equation

$$|\psi\rangle = G^c(E) V_s |\psi\rangle \tag{1.9}$$

where $G^c(E) = (E - H_0 - V_c)^{-1}$. So our task is to find a basis that makes the exact calculation of the matrix elements of the operator G^c and of the vectors $G^c|i\rangle$ possible.

2. PSE method for Coulomb-like potentials

For the sake of simplicity we are concerned in the following with spherical potentials. The radial wavefunction u_l belonging to the lth partial wave satisfies the Lippmann–Schwinger equation

$$u_l(k, r) = \int_0^\infty dr' \, g_l^c(k, r, r') V_s(r') u_l(k, r') \tag{2.1}$$

where $k = [(2m/\hbar^2)E]^{1/2}$ is the wavenumber, $g_l^c(k, r, r')$ is the radial partial wave Coulomb–Green function

$$\langle r | G^c(k) | r' \rangle = \frac{1}{4\pi} \sum_{l=0}^\infty (2l+1) g_l^c(k, r, r') \frac{1}{rr'} P_l(\hat{r} \cdot \hat{r}') \tag{2.2}$$

and $\hat{r}$ is a vector of unit length parallel to r, while P_l is the Legendre polynomial. The radial partial wave Coulomb–Green function can be given in the form

$$g_l^c(k, r, r') = -\varphi_l^c(k, r_<) f_l^c(k, r_>) / \mathscr{F}_l(k) \tag{2.3}$$

where $\varphi_l^c(k, r)$, $f_l^c(k, r)$ and $\mathscr{F}_l(k)$ are the regular Coulomb function, the irregular Coulomb function and the Coulomb–Jost function, respectively, and $r_< = \min(r, r')$, $r_> = \max(r, r')$ (see, e.g., Newton 1982). According to (1.6) and (2.3) the wavefunction $u_l(k_\alpha^N, r)$ is a linear combination of the functions

$$\langle r | g_l^c(k_\alpha^N) | i \rangle \sim \int_0^\infty dr' \, \varphi_l^c(k_\alpha^N, r_<) f_l^c(k_\alpha^N, r_>) \langle r' | i \rangle. \tag{2.4}$$

It can be seen that these functions tend to zero as the regular Coulomb function and tend to infinity as the irregular Coulomb function. That is, the behaviour of the function $\langle r | g_l^c(k_\alpha^N) | i \rangle$ at zero and at infinity is the correct Coulomb-like behaviour. This means that if only the short-range potential is taken in the separable form and equation (1.9) is solved without any further approximation the main advantage of the PSE method is retained, i.e. it gives the wavefunction with correct asymptotics.

The matrix elements of the Coulomb–Green operator between bound state hydrogenic functions have been calculated for describing two-photon processes in a Coulomb field (Zon *et al* 1969) and for calculating the lower bound of an atomic Hamiltonian (Hill and Huxtable 1982). Unfortunately, the bound state hydrogenic functions do not form a complete set. Therefore, we choose another set, which is very similar to the hydrogenic functions: the Coulomb–Sturmian (CS) functions, i.e. the Sturm–Liouville solutions of the hydrogenic problem (Rotenberg 1970, Blinder 1984). In coordinate representation they are given in the form

$$\langle r | nl \rangle = S_{nl}(r) = \left(\frac{n!}{(n+2l+1)!} \right)^{1/2} (2br)^{l+1} e^{-br} L_n^{2l+1}(2br) \tag{2.5}$$

where n goes from zero to infinity, b is a scaling parameter and the functions L_n^{2l+1} are the associated Laguerre polynomials (Erdélyi *et al* 1953). The functions S_{nl} satisfy the differential equation

$$\left(-\frac{d^2}{dr^2}+\frac{l(l+1)}{r^2}-\frac{2b(n+l+1)}{r}+b^2\right)S_{nl}(r)=0 \tag{2.6}$$

and the relations

$$\int_0^\infty dr\, S_{nl}(r)\frac{1}{r}S_{n'l'}(r)=\delta_{nn'}\delta_{ll'} \tag{2.7}$$

$$\sum_{n=0}^\infty S_{nl}(r)S_{nl}(r')=\delta(r-r')(rr')^{1/2} \tag{2.8}$$

i.e. these functions are orthogonal and form a complete set with respect to the weight function $\langle r|\Delta|r'\rangle=\delta(r-r')/r$.

Let us define a new set: $\{|\widetilde{nl}\rangle\}=\{\Delta^{1/2}|nl\rangle\}$. The $|\widetilde{nl}\rangle$ form an orthonormal basis, since

$$\langle\widetilde{nl}|\widetilde{n'l'}\rangle=\langle nl|\Delta|n'l'\rangle=\delta_{nn'}\delta_{ll'} \tag{2.9}$$

$$\sum_{n=0}^\infty|\widetilde{nl}\rangle\langle\widetilde{nl}|=\sum_{n=0}^\infty\Delta^{1/2}|nl\rangle\langle nl|\Delta^{1/2}=1. \tag{2.10}$$

For the sake of an analytical calculation of the matrix elements of the Green operator we rewrite the Lippmann–Schwinger equation. For the vector

$$|\tilde{u}_l\rangle=\Delta^{1/2}|u_l\rangle \tag{2.11}$$

and the operators

$$\tilde{g}_l^c=\Delta^{1/2}g_l^c\Delta^{1/2} \tag{2.12}$$

$$V_s=\Delta^{-1/2}V_s\Delta^{-1/2} \tag{2.13}$$

the Lippmann–Schwinger equation

$$|\tilde{u}_l\rangle=\tilde{g}_l^c V_s|\tilde{u}_l\rangle \tag{2.14}$$

holds.

Let us expand the potential V_s in terms of the basis $\{|\widetilde{nl}\rangle\}$. To construct the Fredholm determinant D, we have to calculate the matrix elements $\langle nl|V_s|n'l'\rangle$ and $\langle nl|\tilde{g}_l^c|n'l'\rangle$. Using the well known recurrence relation of the Laguerre polynomials, we can derive a relation between the neighbouring matrix elements of the operator V_s:

$$[(n+1)(n+l+2)]^{1/2}\langle\widetilde{n+1l}|V_s|\widetilde{n'l'}\rangle-[(n'+1)(n'+l'+2)]^{1/2}\langle\widetilde{nl}|V_s|\widetilde{n'+1l'}\rangle$$
$$=[2(n-n')+4(l-l')]\langle\widetilde{nl}|V_s|\widetilde{n'l'}\rangle-[n(n+2l+1)]^{1/2}\langle\widetilde{n-1l}|V_s|\widetilde{n'l'}\rangle$$
$$+[n'(n'+2l+1)]^{1/2}\langle\widetilde{nl}|V_s|\widetilde{n'-1l'}\rangle. \tag{2.15}$$

This formula tells us that all matrix elements can be derived from the tridiagonal ones, which can always be determined by numerical integration.

Starting from the identity $1=g_l^c\Delta^{-1/2}(E-H_0-V_c)\Delta^{-1/2}$ and using (2.6) and the relationship

$$\langle n'l|nl\rangle=\delta_{nn'}(n+l+1)-\delta_{n',n+1}\frac{1}{2b}[(n+1)(n+2l+2)]^{1/2}-\delta_{n',n-1}\frac{1}{2b}[n(n+2l+1)]^{1/2}$$

$$\tag{2.16}$$

we arrive at a recurrence relation for the vectors $\tilde{g}_l^c|\widetilde{nl}\rangle$

$$
\widetilde{g}_l^c|\widetilde{n+1l}\rangle = \left\{\left[2(n+l+1) - \left(n+l+1+\frac{m}{\hbar^2}\frac{Z_1Z_2e^2}{b}\right)\left(\frac{m}{\hbar^2}\frac{E}{2b}+\frac{1}{4}\right)\right]^{-1}\tilde{g}_l^c|\widetilde{nl}\rangle\right.
$$

$$
\left.-[n(n+2l+1)]^{1/2}\tilde{g}_l^c|\widetilde{n-1l}\rangle - \frac{m/\hbar^2 b}{mE/\hbar^2 2b^2+1/4}|\widetilde{nl}\rangle\right\}
$$

$$
\times[(n+1)(n+2l+2)]^{-1/2} \tag{2.17}
$$

and for the matrix elements $\langle\widetilde{n'l'}|\tilde{g}_l^c|\widetilde{nl}\rangle$

$$
\langle\widetilde{n'l}|\tilde{g}_l^c|\widetilde{n+1l}\rangle = \left\{\left[2(n+l+1) - \left(n+l+1+\frac{m}{\hbar^2}\frac{Z_1Z_2e^2}{b}\right)\left(\frac{m}{\hbar^2}\frac{E}{2b^2}+\frac{1}{4}\right)\right]^{-1}\right.
$$

$$
\times\langle\widetilde{n'l}|\tilde{g}_l^c|\widetilde{nl}\rangle - [n(n+2l+1)]^{1/2}\langle\widetilde{n'l}|\tilde{g}_l^c|\widetilde{n-1l}\rangle
$$

$$
\left.-\frac{m/\hbar^2 b}{mE/\hbar^2 2b^2+1/4}\right\}\delta_{nn'}[(n+1)(n+2l+2)]^{-1/2}. \tag{2.18}
$$

Note that these equations are valid even in case of $n = 0$ so all the matrix elements and functions $\langle r|\tilde{g}_l^c|\widetilde{nl}\rangle$ for the wavefunction can be calculated if $\langle\widetilde{0l}|\tilde{g}_l^c|\widetilde{0l}\rangle$ and $\langle r|\tilde{g}_l^c|\widetilde{0l}\rangle$ are at our disposal.

The matrix element $\langle\widetilde{0l}|\tilde{g}_l^c|\widetilde{0l}\rangle$ can be determined by calculating the double integral

$$
\langle\widetilde{0l}|g_l^c|\widetilde{0l}\rangle = G_{00}^l = \int_0^\infty\int_0^\infty \mathrm{d}r\,\mathrm{d}r'\,S_{0l}(r)g_l^c(r,r')S_{0l}(r')/rr'. \tag{2.19}
$$

By performing the $x = 2br$ and $x' = 2br'$ substitutions and using (2.5), we arrive at the integral

$$
G_{00}^l = \frac{1}{(2l+1)!}\int_0^\infty\int_0^\infty \mathrm{d}x\,\mathrm{d}x'\,\exp\left(-\frac{x+x'}{2}\right)(xx')^l g_l^c(x,x') \tag{2.20}
$$

which is very similar to the integral evaluated by Zon *et al* (1969) and Hill and Huxtable (1982). For future reference we sketch the evaluation of the integral (2.20) following Zon *et al* (1969).

The Coulomb–Green function can be given in the form

$$
g_l^c(x,x') = -\frac{ma\nu}{\hbar^2}\frac{\Gamma(l-\nu+1)}{\Gamma(2l+2)}\mathcal{M}_{\nu,l+1/2}\left(\frac{2x_<}{A\nu}\right)\mathcal{W}_{\nu,l+1/2}\left(\frac{2x_>}{A\nu}\right) \tag{2.21}
$$

where $a = \hbar^2/mZ_1Z_2e^2$, $\nu = 1/ika$, $A = 2ba$ and $\mathcal{M}$ and $\mathcal{W}$ are the regular and irregular Whittaker functions, respectively. Using the integral representation of the product of the Whittaker functions (Buchholz 1969)

$$
\mathcal{M}_{\nu,l+1/2}\left(\frac{2x_<}{A\nu}\right)\mathcal{W}_{\nu,l+1/2}\left(\frac{2x_>}{A\nu}\right)
$$

$$
= \frac{2(xx')^{1/2}}{A\nu}\frac{\Gamma(2l+2)}{\Gamma(l-\nu+1)}\int_0^\infty \mathrm{d}y\,\exp\left(-\frac{x+x'}{A\nu}\cosh y\right)
$$

$$
\times(\coth y/2)^{2\nu}\hat{I}_{2l+1}\left(\frac{2(xx')^{1/2}}{A\nu}\sinh y\right) \tag{2.22}
$$

where $\hat{I}$ is the modified Bessel function of integer order, we can carry out the integration with respect to x' (see Gradshteyn and Ryzhik 1965)

$$G_{00}^l = -\frac{m}{b\hbar^2(2l+1)!} \int_0^\infty \int_0^\infty \int_0^\infty dx\, dx'\, dy\, (xx')^{l+1/2} \exp\left[-\frac{x+x'}{A\nu}\left(\cosh y + \frac{A\nu}{2}\right)\right]$$

$$\times (\coth y/2)^{2\nu} \hat{I}_{2l+1}\left(\frac{2(xx')^{1/2}}{A\nu}\sinh y\right)$$

$$= -\frac{mA\nu}{b\hbar^2(2l+1)!} \int_0^\infty \int_0^\infty dx\, dy\, x^{2l+1} \exp\left(-\frac{x}{A\nu}\frac{1+(\frac{1}{2}A\nu)^2+A\nu\cosh y}{\frac{1}{2}A\nu+\cosh y}\right)$$

$$\times (\sinh y)^{2l+1}(\cosh y/2)^{2\nu}(\tfrac{1}{2}A\nu+\cosh y)^{-2l-2}. \tag{2.23}$$

Now the integration with respect to x and the substitution $t = [\tanh y/2]^{1/2}$ lead to the expression

$$G_{00}^l = -\frac{m}{b\hbar^2}\frac{2^{2l+2}(A\nu)^{2l+3}}{(1+\frac{1}{2}A\nu)^{4l+4}}\int_0^1 dt\, t^{l-\nu}\left[1-\left(\frac{1-A\nu/2}{1+A\nu/2}\right)^2 t\right]^{-2l-2} \tag{2.24}$$

Using the well known integral representation of the $_2F_1$ function (Abramowitz and Stegun 1970) we arrive at the final result

$$G_{00}^l = -\frac{m}{b\hbar^2}\frac{2^{2l+2}(A\nu)^{2l+3}}{(1+A\nu/2)^{4l+4}}\frac{1}{l-\nu+1}\, _2F_1\left(2l+2, l-\nu+1; l-\nu+2; 1-\frac{A\nu}{(1+\frac{1}{2}A\nu)^2}\right) \tag{2.25}$$

The restriction means that the result is valid only on a restricted area of the complex ν or k plane, but it can be continued analytically to the whole complex plane, except for the branch cut from 0 to $-i\infty$, by the aid of the linear transformation formulae of the $_2F_1$ function (Abramowitz and Stegun 1970).

For the calculation of the radial wavefunction (2.1) with the help of (2.17) the knowledge of the function $\langle r|\Delta^{-1/2}\tilde{g}_i^c|\overline{0l}\rangle$ is required. This function can be given by evaluating the interval

$$\langle r|\Delta^{-1/2}\tilde{g}_i^c|\overline{0l}\rangle = \mathscr{F}_0^l = \int_0^\infty dr'\, g_i^c(r, r')\frac{1}{r'}S_{0l}(r')$$

$$= \frac{1}{[(2l+1)!]^{1/2}}\int_0^\infty dx\, g_i^c(x, x')x''\exp\left(-\frac{x'}{2}\right). \tag{2.26}$$

Here we can follow the method used in the calculation of G_{00}^l. Using (2.22) the integral can be given in the form

$$\mathscr{F}_0^l = -\frac{m}{\hbar^2 b[(2l+1)!]^{1/2}}\int_0^\infty \int_0^\infty dx'\, dy\, x^{1/2}\exp\left(-\frac{1}{A\nu}[\tfrac{1}{2}A\nu x' + (x+x')\cosh y]\right)$$

$$\times (\coth y/2)^{2\nu}x''^{l-1/2}\hat{I}_{2l+1}\left(\frac{2(xx')^{1/2}}{A\nu}\sinh y\right). \tag{2.27}$$

The integration with respect to x' can be performed in a way similar to (2.23). With the substitution

$$t = (1-\tanh^2 y/2)\left(1+\frac{1-A\nu/2}{1+A\nu/2}\tanh^2 y/2\right)^{-1}$$

and with the notation $\xi = (1 - A\nu/2)/2$ we arrive at the formula

$$\mathcal{F}_0^l = -\frac{m}{b\hbar^2[(2l+1)!]^{1/2}} \frac{A\nu}{1+A\nu/2} \exp\left(-\frac{x}{A\nu}\right) q(x) \tag{2.28}$$

where

$$q(x) = \int_0^1 dt \exp\left(\frac{2x}{A\nu}\xi(1-t)\right)(1-t)^{l-\nu}\left(1-\frac{\xi}{\xi-1}t\right)^{l+\nu}. \tag{2.29}$$

Expanding the exponential function into a power series we have

$$q(x) = \int_0^1 dt\,(1-t)^{l-\nu}\left(1-\frac{\xi}{\xi-1}t\right)^{l+\nu} + \frac{2x\xi}{A\nu}\int_0^1 dt\,(1-t)^{l-\nu+1}\left(1-\frac{\xi}{\xi-1}t\right)^{l+\nu}$$

$$+\frac{(2x\xi/A\nu)^2}{2!}\int_0^1 dt\,(1-t)^{l-\nu+2}\left(1-\frac{\xi}{\xi-1}t\right)^{l+\nu} + \dots \tag{2.30}$$

Conferring this with the integral representation of the $_2F_1$ function we obtain a series

$$q(x) = {}_2F_1\left(-l-v, 1; l-\nu+2; \frac{\xi}{\xi-1}\right)(l-\nu+1)^{-1}$$

$$+\frac{2x\xi}{A\nu}\,{}_2F_1\left(-l-\nu, 1; l-\nu+3; \frac{\xi}{\xi-1}\right)(l-\nu+2)^{-1}$$

$$+\frac{(2x\xi/A\nu)^2}{2!}\,{}_2F_1\left(-l-\nu, 1; l-\nu+4; \frac{\xi}{\xi-1}\right)(l-\nu+3)^{-1} + \dots \tag{2.31}$$

in which the consecutive hypergeometric functions differ only in one index, so they can be calculated via a recurrence relation of Abramowitz and Stegun (1970) provided the first two functions are known. Of course this result is valid only on a very restricted area of the complex plane but it can be continued analytically.

The matrix elements of the operator $\tilde{g}_l^{c^2}$ needed for the normalisation of the wavefunction are determined by the aid of the well known operator identity

$$\tilde{g}_l^{c^2}(E) = -\frac{d}{dE}\,\tilde{g}_l^c(E). \tag{2.32}$$

Starting from the matrix elements of the operator $\tilde{g}_l^c$ we approximate the derivative with a finite difference.

3. Numerical results

To demonstrate the feasibility of the method, we present the energy and wavefunction of a resonant state, for which the asymptotics is more crucial than for a bound state. In our example a proton with quantum numbers $l = 4$, $j = \frac{9}{2}$ moves in the field of a nucleus represented by a spherical Coulomb-like potential. The V of (1.8) has the form

$$V = V_0 f(r) + V_{so}\left(\frac{\hbar^2}{m_\pi c}\right)^2 \frac{1}{r}\frac{df(r)}{dr}l\sigma + V_{cl} \tag{3.1}$$

with

$$f(r) = -\{1 - \exp[(r - R_0)/d]\}$$

and

$$V_{cl} = \begin{cases} Z_1 Z_2 (e^2/2R_c)(3 - r^2/R_c^2) & r < R_c \\ Z_1 Z_2 e^2/r & r > R_c. \end{cases}$$

The parameter values $V_0 = 50.9$ MeV, $V_{so} = 5.8$ MeV, $R_0 = R_c = 7.06$ fm, $d = 0.75$ fm, $Z_1 = 82$, $Z_2 = 1$ and $b = 2.69$ fm^{-1} were chosen. For comparison the exact numerical solution was determined with the code of Vertse *et al* (1982). Table 1 shows the convergence of the energy as a function of N. The exact value is $(13.57 - 0.34i)$ MeV. In figure 1 the wavefunction belonging to $N = 19$ is shown. The agreement is excellent, the difference between the PSE and exact wavefunction cannot be displayed in the figure, the relative error being everywhere less than 0.01.

We have found that the rate of convergence depends weakly on the parameter b of CS functions. The optimal parameter b is influenced mainly by the extent of the potential, so it can be scaled with a characteristic length parameter of the potential. In potentials, which are similar to our example, the optimal b is around $19/R_0$.

Table 1. The convergence of the PSE energy of the proton resonance with quantum numbers $l = 4$, $j = \frac{9}{2}$ in the potential (3.1). A scaling parameter $b = 2.69$ fm^{-1} was chosen. The exact energy is $(13.57 - 0.34i)$ MeV.

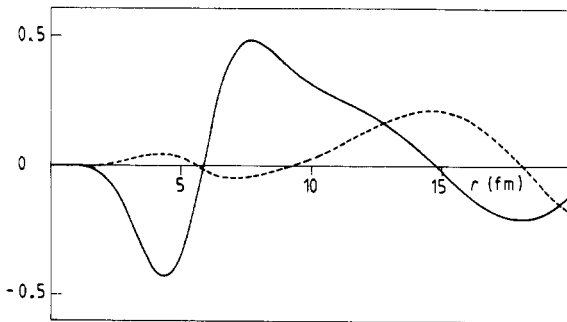| N	
10	$13.330 - 0.321i$
11	$13.581 - 0.308i$
12	$13.621 - 0.328i$
13	$13.592 - 0.356i$
14	$13.570 - 0.356i$
15	$13.567 - 0.341i$
16	$13.571 - 0.336i$
17	$13.573 - 0.338i$
18	$13.573 - 0.340i$
19	$13.571 - 0.340i$

Figure 1. The radial wavefunction belonging to the state in table 1 with $N = 19$. The full and broken curves represent the real and imaginary part of the wavefunction, respectively.

4. Discussion

In this paper we have generalised the potential separable expansion method to calculating bound and resonant states in Coulomb-like potentials. We pointed out that the long-range part of the potential should not be truncated if we want to get a wavefunction with correct asymptotics. In this case the calculation of the matrix elements of the Coulomb–Green operator is required, but this seems to be hopeless in closed form if an HO basis is used.

Attached to the fully elaborated (Kruppa and Papp 1985) HO formalism Gyarmati and Kruppa (1986) truncated the whole Coulomb-like potential, thus giving up the correct Coulomb asymptotics. To reach convergence they render the size parameter of the HO functions complex. However, due to the adequate treating of the Coulomb tail we could reach convergence in the same example on a considerably smaller basis.

Summarising our results we can say the following. We succeeded in finding a basis, which makes the exact calculation of the Coulomb–Green operator possible. These Coulomb-Sturmian functions have a very simple form both in coordinate and momentum representation. The relationship among the matrix elements of the potential reduces the number of matrix elements to be calculated numerically. We have found simple recurrence relations for the matrix elements of Coulomb–Green operator and for the action of this operator on the CS functions. The starting points of these recurrence relations can be given in closed forms so, to calculate resonances, both of them can be continued analytically. We can say that the PSE method based on CS functions shares most of the advantages of that based on the HO functions and it gives wavefunctions with the correct asymptotics not only for short-range but also for Coulomb-like potentials.

From the computational point of view this method can also compete with the HO based method. We have found that the code give the same results for double and extended precision. This means that the whole procedure is computationally well conditioned and the recurrence relations are sufficiently stable.

There are numerous methods for bound state calculations in a Coulomb-like potentials but only few for Gamow states. The main advantage of our method over most of the others is that it can easily be extended to complicated systems, for example for those which have been solved so far with the HO based PSE method for short-range potentials.

References

Abramowitz M and Stegun I A 1970 *Handbook of Mathematical functions* (New York: Dover) ch 15
Berggren T 1968 *Nucl. Phys.* A **109** 265
Blinder S M 1984 *Phys. Rev.* A **29** 1674
Buchholz H 1969 *The Confluent Hypergeometric Functions* (Berlin: Springer) p 86

Erdélyi A, Magnus W, Oberhettinger F and Tricomi F G 1953 *Higher Transcendental Functions* vol II (New York: McGraw-Hill) p 188

Gareev F A, Ershov S N, Révai J, Bang J and Nillsson B S 1979 *Phys. Scr.* **19** 509

Gareev F A, Gizzatkulov M Ch and Révai J 1977 *Nucl. Phys.* A **286** 512

Gradshteyn I S and Ryzhik I M 1965 *Table of Integrals, Series and Products* (New York: Academic) formula 6.643.4

Gyarmati B and Kruppa A T 1982 *Nucl. Phys.* A **378** 407

—— 1986 *Phys. Rev.* C **34** 95

Gyarmati B, Kruppa A T, Papp Z and Wolf G 1984 *Nucl. Phys.* A **417** 393

Gyarmati B, Kruppa A T and Révai J 1979 *Nucl. Phys.* A **326** 119

Hill R N and Huxtable B D 1982 *J. Math. Phys.* **23** 2365

Kruppa A T and Papp Z 1985 *Comput. Phys. Commun.* **36** 59

Newton R G 1982 *Scattering Theory of Waves and Particles* (Berlin: Springer) ch 14.6

Pál K F 1985 *J. Phys. A: Math. Gen.* **18** 1665

Révai J 1975 *E4-9429 Preprint* JINR, Dubna

Révai J, Sotona M and Žofka J 1985 *J. Phys. G: Nucl. Phys.* **11** 745

Rotenberg M 1970 *Adv. At. Mol. Phys.* **6** 233

Truhlik E 1978 *Nucl. Phys.* A **296** 134

Vertse T, Pál K F and Balogh Z 1982 *Comput. Phys. Commun.* **27** 309

Zon B A, Manakov N L and Rapoport L P 1969 *Sov. Phys.–JETP* **28** 480