Theor Chim Acta (1989) 75: 223-232

Theoretica Chimica Acta

Rapidly converging threshold value calculations in screened coulomb potential systems: Critical values of the screening parameter for the Yukawa case

Metin Demiralp

Tübitak, Research Institute for Basic Sciences, Applied Mathematics Department, P.O. Box 74, 41470 Gebze Kocaeli, Turkey

(Received December 27, 1987; revised February 11/Accepted February 26, 1988)

In this work, the threshold values of the screening parameter for Yukawa potential systems are obtained by means of a basis set constructed from Laguerre type functions. The Laguerre basis set is modified by an appropriately chosen extra function in order to imitate the true behaviour of the solutions at the boundary points. The method used is a variational scheme and the numerical results are accurate to thirty decimal points. A scaling parameter is also inserted into the structure of the basis functions, the optimized values of which accelerate the convergence. The main goal of this paper is to develop a method which enables us to calculate the threshold values of the screening parameter for low-lying states. The method is quite general and can be extended to all systems whose potentials decay exponentially when the radial variable goes to infinity.

Key words: Screened coulomb potentials — Yukawa potentials — Variational methods — Threshold value calculations

1. Introduction

In this work, the direct calculation of the threshold values of screening parameters in screened coulomb potential systems is presented. This becomes important when we deal with physical phenomena like collision, excitation, ionization, scattering etc., due to the fact that one needs to know when a state of the discrete spectrum transforms into a state of the continuous spectrum as the screening parameter increases. Indeed, the existence of screening in a coulombic potential reduces the number of possible bound states to a finite one whose value is completely determined by the value of the screening parameter and by the type of the screening potential. Therefore, the possibility of scattering or ionization increases and the bond strength between the particles diminishes as the screening

parameter value increases. In certain type of scattering calculations the number of bound states must be known. However, this is only possible when we know the accurate threshold values of the screening parameter where the bound state under consideration can not survive anymore.

Most of the common methods become incapable of obtaining sufficiently accurate energy eigenvalues when the screening parameter approaches its threshold value. However, if the threshold values of the screening parameter can be calculated within sufficient accuracy then one is able to expand energy eigenvalues in powers of the difference between the screening parameter and its threshold value. The common approach is to perform energy eigenvalue calculations for increasing values of the screening parameter until the resulting energy value vanishes within the desired precision [1–3]. This is of course, a cumbersome process and furthermore it is very sensitive to numerical error accumulations. As a matter of fact, most of the well-known methods for eigenvalue calculations tend to converge slowly around the continuous spectrum threshold and necessitate many more iteration steps. Therefore, we have to seek an efficient way which enables us to find the threshold values of the screening parameter directly. The screening parameter appears as a scaling factor in the structure of screened coulomb potentials. This enables us to convert the Schroedinger equation to a generalised eigenvalue problem by replacing the energy parameter with zero and by rescaling the radial coordinate. The resulting problem has a weight which is merely the potential term, and its spectral behaviour is quite different from that of the original Schroedinger equation. In fact, it seems to have only a discrete spectrum, although we are not going to attempt to give a detailed proof of this.

Before proceeding, let us mention our assumptions to facilitate certain intermediate steps of our calculations. First of all, we are interested only in radially screened coulomb potential systems. Since these are frequently employed as successful models to describe many physical or chemical phenomena [4–6], this is not a serious restriction. Although it is possible to import the angular dependence through the screened part of the coulombic potential, we are not going to deal with this. Moreover, we shall confine ourselves to the specific case where the potential is of Yukawa type [7–11]. However, the discussions and applications presented here are quite generalisable to any angle-independent potentials which decay exponentially when the radial variable tends to infinity.

The solution of the generalised eigenvalue problem to produce the threshold values of the screening parameter can be accomplished with the aid of various methods like variational approaches, perturbational techniques, resolvent operator methods etc. Since the use of perturbational techniques necessitates a good choice of an unperturbed operator and we do not have sufficient insight to this end, we prefer to utilise a variational scheme.

As is well-known, the most important thing in the use of variational schemes is the construction of an efficient basis set. Indeed, the basis functions which imitate the main features of the true solution yield high precision results with a minimum computational effort. On the other hand variational schemes give the eigenvalues

starting from the smallest (largest) when the operator under consideration is bounded below (above). Therefore, the variational calculation of the highly excited state eigenvalues increases the necessary computational effort and becomes impossible after a specific eigenvalue depending on the nature of the computational facilities used in the calculation. Hence this approach is incapable of obtaining the entire spectrum. However, many physical and chemical phenomena deal with only the low-lying states of the system. So, we are going to leave the calculation of the entire spectrum of screening parameter threshold values and try to obtain several low-lying state threshold values for Yukawa potential systems.

In the frame of this discussion the second section of this paper will be dedicated to the presentation of the basis set construction for the variational scheme, where analytical formulae for the calculation of matrix elements will be presented. The third section covers the numerical results for the Yukawa case with a sufficient discussion about the details of computation. The last section will include the concluding remarks.

2. Basis set construction for the variational scheme

If we consider the Schroedinger equation for a central field potential, we can write the following equation after the seperation of angular behaviour as a factor of spherical harmonics

$$\left[-\frac{1}{2}\frac{d^2}{dr^2}-\frac{1}{r}\frac{d}{dr}+\frac{l(l+1)}{2r^2}-\frac{V(\gamma r)}{r}\right]\psi = E\psi \tag{2.1}$$

where Hartree units are used. l and γ denote the azimuthal quantum number and screening parameter respectively. The function V is responsible for the screening of the pure coulomb field. It is assumed to be unity when r vanishes without any loss of generality since a scaling transformation donates this property to it. The accompanying boundary conditions necessitate that V must be continuous for all possible r values and must have sufficiently rapid decay to be included in a square integrable function set under the weight r^2.

Of course, V might be a function of angles, however at this stage, the introduction of this complication is unnecessary, since we are interested, at first, in finding the most efficient way for the calculation of screening parameter threshold values, in rather simple cases.

As we know, the Eq. (2.1) becomes the Schroedinger equation for the hydrogen atom when γ vanishes. Therefore, if we trace the energy dependence on γ values for a specific bound state, we see that it starts from the corresponding hydrogenic state and arrives at the threshold of the continuum where the energy is zero after a monotonic increase in value. We call the value of the screening parameter at this point as its "threshold value". Hence by setting E equal to zero in Eq. (2.1) and by replacing γr with r for a rescaling transformation we can obtain

$$\left[-\frac{d^2}{dr^2}-\frac{2}{r}\frac{d}{dr}+\frac{l(l+1)}{r^2}\right]\psi_{cr} = \frac{2}{\gamma}\frac{V(r)}{r}\psi_{cr}; \qquad \gamma > 0. \tag{2.2}$$

Since ψ_{cr} belongs to the set of functions which are square integrable with respect to the weight r^2, the first thing that comes to mind is to employ the following weighted polynomials $P_{n-1}^{(l)}$ as basis functions with a normalisation constant A_n

$$\varphi_n = A_n r^l e^{-sr} P_{n-1}^{(l)}(\sigma r) \tag{2.3}$$

where the parameters s and σ are introduced to give the flexibility of affecting the convergence rate of the variational procedure. As we can immediately notice, the application of the variational scheme via a trial function which is formed as a linear combination of given basis functions yields a matrix eigenvalue equation with a non-unit matrix weight, unless the given basis functions are orthonormal with respect to the weight function $V(r)/r$. On the other-hand $V(r)/r$ can be considered as a weight function only when it is positive for all values of r, otherwise the positive definiteness of the corresponding weight matrix is not guaranteed for all finite linear combinations of basis functions. This means, the conversion of the weight matrix to unit matrix via a suitable matrix transformation is not always possible. As a matter of fact, we could use the left hand side operator in Eq. (2.2) as a weight operator. Since it is positive definite, it would permit us to convert its truncated matrix representation to a unit matrix. However, this procedure, possibly necessitates the construction of a new orthonormal polynomial set. Henceforth, we assume that $V(r)/r$ is positive for all r values. Under this assumption $P_{n-1}^{(l)}$ polynomials can be constructed from the set of functions $(1, r, r^2, \ldots)$ via the Gramm-Schmidt orthonormalisation procedure by using $V(r)/r$ as weight in the integral of the scalar product. Of course this orthonormalisation may be considered unnecessary. However, if it is not carried out, the resulting weighted matrix eigenvalue problem becomes numerically open to error accumulations coming from the extra diagonalisation of the weight matrix. In fact, there is a hidden numerical orthonormalization procedure in the solution of generalised matrix eigenvalue problems. Hence the solution of the unit weight matrix eigenvalue problems must be preferred instead of the above one.

In this work, we specify $V(r)$ as follows

$$V(r) = e^{-r} \tag{2.4}$$

to avoid dealing with the construction of certain unusual polynomials and to benefit from the advantages of using Laguerre polynomials. Furthermore, this specification confines us to Yukawa potential systems which still preserves their attractiveness in both physical and mathematical senses. So we can use the following quite standard functions as a basis set

$$\varphi_n = \left[\frac{(n-1)!}{(n+2l)!}\right]^{1/2} (1+2s)^{l+1} r^l e^{-sr} L_{n-1}^{2l+1}((1+2s)r) \tag{2.5}$$

where L_{n-1}^{2l+1} denotes the associated Laguerre polynomials. These functions are orthonormal with respect to the weight e^{-r}/r and contain only one adjustable parameter. Although we are not going to present the results, the variational scheme via these basis functions does not produce rapidly converging values, even when the adjustable parameter, s is optimised. This is mainly due to the

lack of the reflections of the true eigenfunction behaviours especially at the endpoints of r-interval. Therefore, we can attempt to cure this weakness of the basis functions, using the following finite set of basis functions

$$\phi_n = \varphi_n; \qquad n = 1, 2, \ldots, N-1 \tag{2.6}$$

$$\phi_N = B\left\{ C(1-e^{-sr}\xi_{2l}(sr))/r^{l+1} - \sum_{n=1}^{N-1} q_n \varphi_n \right\} \tag{2.7}$$

$$\xi_{2l} = \sum_{j=0}^{2l} \frac{s^j r^j}{j!} \tag{2.8}$$

where B, C and q_n are to be determined through the following conditions to fulfill the requirements of the Gram-Schmidt procedure

$$C^2 \int_0^\infty r^{-2l-1} e^{-sr}[1-e^{-sr}\xi_{2l}(sr)]^2 \, dr = 1 \tag{2.9}$$

$$q_n = C \int_0^\infty \varphi_n (1-e^{-sr}\xi_{2l}(sr)) \, e^{-r} r^l \, dr \tag{2.10}$$

$$B = \left[1 - \sum_{k=1}^{N-1} q_n^2 \right]^{1/2} \tag{2.11}$$

where the summations whose upper index is smaller than their lower one are assumed to vanish. By performing the necessary integrations we can arrive at the following analytical results

$$C = [(2l)!]^{1/2}[C_1 + C_2 - C_3 + C_4]^{1/2} \tag{2.12}$$

$$C_1 = 2\ln(1+s) - \ln(1+2s) \tag{2.13}$$

$$C_2 = \sum_{k=0}^{2l-1} \frac{(-s)^{k+1}}{(k+1)} \tag{2.14}$$

$$C_3 = (1+s)^{2l} \sum_{j=0}^{2l} \sum_{k=0}^{2l-j-1} \binom{2l-1-k}{j} \frac{1}{(k+1)} \left(-\frac{s}{1+s} \right)^{j+k+1} \tag{2.15}$$

$$C_4 = (1+s)^{2l} \sum_{j=0}^{2l} \left(-\frac{s}{1+s} \right)^j \sum_{k=0}^{j-1} \frac{1}{j-k} \binom{2l-j+k}{k} \left(\frac{s}{1+2s} \right)^{j-k} \tag{2.16}$$

$$q_n = \left[\frac{(n-1)!}{(n+2l)!} \right]^{1/2} (1+2s)^{l+1} C \left[\frac{d_1}{1+s} - \frac{d_2}{1+2s} \right] \tag{2.17}$$

$$d_1 = \sum_{m=0}^{n-1} \binom{2l+m}{m} \left(-\frac{s}{1+s} \right)^{n-m-1} \tag{2.18}$$

$$d_2 = \sum_{m=0}^{2l} \binom{2l-m+n-1}{n-1} \left(\frac{s}{1+2s} \right)^m. \tag{2.19}$$

These form the recipe for the matrix element calculations in the variational scheme. Let us, now, discuss the selection of the function given by Eq. (2.7) and the linear independence of the set given by Eqs. (2.7) and (2.8)

Since the threshold values are relevant to the behaviour of system's wave functions at infinity, we must reflect the true eigenfunction's behaviour at infinity in the trial function. Due to the exponential decay in V when r goes to infinity, the solutions of the Eq. (2.2) must asymptotically approach the decaying homogeneous solution for the radial part of the Laplace operator. Therefore

$$(\psi_{cr})_{r\to\infty} = C/r^{l+1}. \tag{2.20}$$

This, however, implies that the trial function must have the following form

$$\psi_T = C[r^{-l-1} - \eta(r)] \tag{2.21}$$

where $\eta(r)$ is an exponentially decaying function.

On the other hand, attempts to obtain the formal solution of the Eq. (2.2) around its regular singular point where $r=0$, show that the true eigenfunction must behave like r^l when r tends to vanish. Hence we can write

$$\psi_T = Cr^{-l-1}[1 - e^{-sr}\xi_{2l}(sr)] + C\eta_1(r) \tag{2.22}$$

where $\eta_1(r)$ is analytic everywhere and exponentially decays at infinity. Therefore, we have verified the selection given by Eq. (2.7).

As a matter of fact, ϕ_N and the φ_n-functions can not stay linearly independent as N increases unboundedly. Since any function which is regular for all r values except certain finite jumps at a finite number of points in the domain of r, can be expanded into an infinite series of φ_n-functions. This expansion converges in the mean, everywhere except at singular points. This linear dependence is unavoidable. However, for finite N values they remain linearly independent for an appropriate choice of the s value.

3. Numerical applications for Yukawa case

If we consider the following matrix elements

$$H_{jk} = \int_0^\infty \phi_j \left[-\frac{d^2}{dr^2} - \frac{2}{r}\frac{d}{dr} + \frac{l(l+1)}{r^2} \right] \phi_k \, dr \tag{3.1}$$

we can formulate the eigenvalue problem resulting from the variational scheme as follows

$$\boldsymbol{Ha} = (2/\gamma)\boldsymbol{a} \tag{3.2}$$

where $\boldsymbol{a}$ is an N-dimensional vector whose elements are merely the linear combination coefficients appearing in the trial function. Now, we need the values of the elements of H to perform necessary numerical steps. To this end, we can write the following equation

$$\left[-\frac{d^2}{dr^2} - \frac{2}{r}\frac{d}{dr} + \frac{l(l+1)}{2r^2} \right] \varphi_k = \left[\frac{2s(k+1)}{r} - s^2 \right] \varphi_k + \frac{[(k+2l)(k-1)]^{1/2}}{r} \varphi_{k-1} \tag{3.3}$$

after using certain formulae for Laguerre polynomials. This, however, implies that

$$H_{jk}=2s(k+l)G_{jk}+[(k+2l)(k-1)]^{1/2}G_{jk-1}-s^2\int_0^\infty \varphi_j\varphi_k\,dr,$$
$$1\leq j,\,k\leq N \qquad (3.4)$$

where

$$G_{jk}=\int_0^\infty \varphi_j\varphi_k\frac{dr}{r}. \qquad (3.5)$$

If we use the following formula which is derived from the recursion formula for Laguerre polynomials

$$(1+2s)r\varphi_k=-[k(k+2l+1)]^{1/2}\varphi_{k+1}+(2k+2l)\varphi_k$$
$$-[(k-1)(k+2l)]^{1/2}\varphi_{k-1} \qquad (3.6)$$

we can write

$$\int_0^\infty \varphi_j\varphi_k\,dr=\frac{1}{(1+2s)}\{-[k(k+2l+1)]^{1/2}G_{jk+1}+(2k+2l)G_{jk}$$
$$-[(k-1)(k+2l)]^{1/2}G_{jk-1}\}. \qquad (3.7)$$

Therefore, the evaluation of the G_{jk}^{-} terms is sufficient for the determination of the H_{jk}-elements. This, however, can be accomplished by repetitive use of Eq. (3.6) arriving at the following two-index recursion [11].

$$G_{j+1k}=[j(j+2l+1)]^{1/2}\{[k(k+2l+1)]^{1/2}G_{jk+1}+[(k-1)(k+2l)]^{1/2}G_{jk-1}$$
$$-[(j-1)(j+2l)]^{1/2}G_{j-1k}+2(j-k)G_{jk}\},\qquad j,\,k=1,2,\ldots. \qquad (3.8)$$

Therefore, we need only know the elements whose first (or second) index is one, to evaluate all G-terms. Since an $M\times M$ array of G-terms necessitates the evaluation of the first $2M$ elements in the first row (column) of the G-table (a two-dimensional array), the evaluation of the M-dimensional H matrix can be realised by a knowledge of the first $(2M+2)$-terms in the first row of the G-table. Therefore, to complete the variational matrix calculation we need only the following formula

$$G_{1k}=\frac{(1+2s)^{2l+2}}{(2l+1)!}[(k-1)!]^{1/2}\int_0^\infty r^{2l+1}\,e^{-2sr}L_k^{2l+1}((1+2s)r)\,dr$$
$$=\binom{k+2l+1}{k}\frac{[(k-1)!]^{1/2}(1+2s)^{2l+2}}{(-2s)^{k+2l+2}} \qquad (3.9)$$

which is obtained after performing certain integrations over Laguerre polynomials [12].

So, we are now able to solve numerically the finite dimensional matrix eigenvalue problems resulting from the variational scheme. The execution of the numerical computations is realised for several dimensions and scaling parameter values.

Table 1. Threshold values of the screening parameter for the Yukawa potential system in descending order

State	Threshold value									
1*s*	1.190	612	421	060	617	705	342	777	106	361
2*s*	0.310	209	282	713	936	939	110	112	212	953
2*p*	0.220	216	806	606	573	040	405	041	463	290
3*s*	0.139	450	294	064	178	013	882	357	954	890
3*p*	0.112	710	498	359	524	944	973	972	952	155
3*d*	0.091	345	120	771	732	184	927	710	066	860
4*s*	0.078	828	110	273	171	565	170	282	204	980
4*p*	0.067	885	376	100	579	552	788	417	968	578
4*d*	0.058	105	052	754	469	264	181	224	714	848
5*s*	0.050	583	170	374	558	799	782	284	408	668
4*f*	0.049	831	132	318	645	225	242	887	831	002
5*p*	0.045	186	248	071	624	990	093	706	122	691
5*d*	0.040	024	353	938	324	274	958	258	960	951
5*f*	0.035	389	389	799	948	414	321	063	141	283
6*s*	0.035	183	477	367	820	588	148	390	875	853
6*p*	0.032	174	932	293	205	003	538	581	132	480
5*g*	0.031	343	552	436	538	045	217	407	715	656
6*d*	0.029	166	650	229	397	650	381	902	551	150
6*f*	0.026	350	671	639	829	827	843	633	383	329
7*s*	0.025	876	416	481	121	578	169	930	945	718
7*p*	0.024	047	639	235	996	140	851	390	943	514
6*g*	0.023	799	103	968	969	544	816	131	058	183
7*d*	0.022	161	826	355	339	786	360	688	903	637
6*h*	0.021	524	548	401	894	416	262	524	364	337
7*f*	0.020	342	170	661	307	635	762	223	228	439
8*s*	0.019	826	307	429	825	264	337	059	425	553
7*g*	0.018	646	215	359	623	339	252	011	442	697
8*p*	0.018	640	705	347	623	634	654	280	763	092
8*d*	0.017	390	648	079	030	682	359	871	838	426
7*h*	0.017	095	135	615	471	857	578	885	041	702
8*f*	0.016	156	534	483	956	706	186	410	014	683
7*i*	0.015	691	083	667	701	475	990	456	076	173
9*s*	0.015	673	723	828	474	905	372	994	735	928
8*g*	0.014	980	862	636	386	665	583	951	297	415
9*p*	0.014	865	869	356	224	286	239	220	545	742
9*d*	0.013	999	880	572	892	515	518	358	979	692
8*h*	0.013	883	519	722	165	163	911	660	037	295
9*f*	0.013	129	670	383	752	190	264	262	157	895
8*i*	0.012	871	464	312	728	093	468	171	298	690
10*s*	0.012	700	950	763	810	386	771	388	389	902
9*g*	0.012	286	145	678	137	967	681	387	938	966
10*p*	0.012	128	229	513	755	452	397	915	667	880
8*j*	0.011	944	531	306	208	677	525	206	756	337
10*d*	0.011	506	513	742	042	353	053	318	933	727

The scaling parameter s is chosen such that one-dimensional matrix eigenvalue problem produces the minimum value of its eigenvalue. Here we did not use an exact minimisation procedure to avoid unnecessary effort. As a matter of fact,

Table 2. Variation of the linear independence parameter with respect to dimension and scaling parameter

l	s	M	N	$B\times10^{-N}$
0	1	20	13	2.07516
0	1	40	26	9.50772
0	1	60	34	−5.77779
0	3	20	6	1.31374
0	3	40	12	6.78391
0	3	60	23	4.59198
0	6	20	4	2.66292
0	6	40	7	2.94265
0	6	60	10	4.19869
0	6	80	13	6.67860
4	1	20	19	6.20593
4	1	40	27	−5.34421
4	5	20	10	2.55224
4	5	40	16	8.56035
4	5	60	20	2.16130
4	5	80	24	1.33504
4	13	40	12	5.77526
4	13	80	17	5.87749
8	10	40	17	1.38541
8	10	80	23	−1.10530
8	20	40	16	6.05098
8	20	80	21	5.52247

l: azimythal quantum number; M: dimension of the subspace spanned by Laguerre polynomials; s: scaling parameter; B: linear independence parameter

determination of the scaling parameter becomes a cumbersome procedure when the dimension of the variational scheme increases. Hence we have taken a reasonable value of s, and tried to increase the dimension of the variational scheme until the desired accuracy is obtained. However, to stabilise the excited states we have had to increase the s-values. This increase necessitates an increase in dimension.

Results for threshold values of γ are presented in Table 1 in descending order. Usual spectroscopical notation is used to specify the states ($s, p, d, f, g, h, i, j, \ldots$). These results are obtained using dimensions between forty and a hundred and scaling parameter values changing from 1.5 for the $1s$-state to 15.0 for the highest excited state given in table. 30-digit precision is given there, however the last decimal point may have an error of ±1. A VAX11/780 computer is used in computations and FORTRAN programmes are run in quadruple precision. The standard routines TRED2 to tridiagonalise the symmetric variational matrix and TQL2 to solve the eigenvalue problem of resulting tridiagonal matrix [13] were employed.

In Table 2, the reciprocal of B^2 in Eqs. (2.7) and (2.11) is used as a measure of the linear independence of ϕ_N and $\{\varphi_1, \ldots, \varphi_{N-1}\}$. Its values are given for several

independence can be strengthened by increasing the value of s as the state number and the dimension of variational scheme increase. Therefore, it can be used as a criterion in the selection of a suitable s. If s is not chosen in the vicinity of its values which increases the linear independence, then numerical error accumulation, hence an oscillating character, in the last decimal points of the threshold value appears.

4. Concluding remarks

In this work, we have calculated threshold values of the screening parameter for certain low-lying states of Yukawa potential systems. Although a variational scheme has been used, we have introduced a novel basis set instead of standard ones. Quite accurate results are obtained after an appropriate selection of scaling parameter. However, as is expected from all variational schemes, it is not possible to evaluate any desired, say hundredth, eigenvalue within a prescribed accuracy. This can possibly be accomplished by using perturbational schemes as we plan for future work. The next step of our studies will be the development of the asymptotic formulae for the energy eigenvalue calculations in Yukawa potential systems. This can be successfully realised only after the present work has been completed. So, we now have a sufficient tool for this purpose. The restriction about the type of screened coulomb potential is not very serious. As a matter of fact, one can easily generalise the concepts and the criteria in the construction of the basis set to the more general screened coulomb potentials which decay exponentially at infinity. On the other hand if the potential does not decay exponentially, then certain modifications may be necessary. Therefore, as a conclusion, we have all appearances of the possibilities to accurately calculate the values at the threshold regimes in screened coulomb potentials.

Acknowledgement. I thank Dr. N.A. Baykara for his careful reading of the manuscript and his several comments about the presentation of the work.

References

1. Rogers FJ, Graboske HC, Harwood DJ (1970) Phys Rev A1:1577
2. Lai CS (1981) Phys Rev 23:455
3. Cizek, J, Vrscay ER (1982) Int J Quantum Chem 21:27
4. Gazeau JP, Maquet A (1979) Phys Rev A20:727
5. Yukawa M (1835) Proc Soc Jpn 17:48
6. Pratt RH, Tsena HK (1972) Phys Rev A5:1063
7. McEnnan J, Kissel L, Pratt RH (1976) Phys Rev A13:532
8. Vrscay ER (1986) Phys Rev A33:1433
9. Adams BG, Cizek J, Paldus J (1982) Int J Quantum Chem 21:153
10. Taseli H, Demiralp M (1987) Theor Chim Acta 71:315
11. Demiralp M, Baykara NA, Taseli H (1988) Convergent perturbation studies in screened coulomb potential systems: a high precision numerical algorithm via Laguerre basis set. Theor Chim Acta 74:39–54
12. Gradshteyn IS, Ryzhik IM (1965) Table of integrals, series and products. Academic Press, New York
13. Press HW, Flannery BP, Teukolsky SA, Vetterling WT (1986) Numerical recipes. Cambridge University Press, Cambridge