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1991 J. Phys. A: Math. Gen. 24 2061

(http://iopscience.iop.org/0305-4470/24/9/016)

J. Phys. A: Math. Gen. 24 (1991) 2061-2068. Printed in the UK

Critical screening parameters for screened Coulomb potentials*

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Received 19 November 1990

Abstract. We develop a simple numerical method to integrate one-dimensional eigenvalue equations and apply it to the calculation of critical screening parameters for screened Coulomb potentials. The method is based on the propagation matrix for the solutions of the eigenvalue equation and its accuracy is easily and systematically improved provided the coefficients of the eigenvalue equation can be expanded in a Taylor series about every point of the grid. We show results for the static screened and exponential cosine screened Coulomb potentials.

1. Introduction

Screened Coulomb potentials prove to have many physical applications [1-3]. Among such models we mention the static screened and exponential cosine screened Coulomb potentials (SSC and ECSC potentials, respectively) which have been widely discussed lately [4, 5]. They can be written as

$$V(r) = -r^{-1}\cos(\varepsilon\delta r)\,\mathrm{e}^{-\delta r} \tag{1}$$

where $\varepsilon = 0$ and 1 in the former and latter cases, respectively. Throughout this paper atomic units are used.

The most important quantities of interest regarding these potentials are either the number of bound states or the critical screening parameter [1]; the latter being the δ value for which the value of the largest bound-state energy level is exactly zero. Critical screening parameters have been obtained by Rogers *et al* [1] and Singh and Varshni [5] using numerical integration algorithms and by Kesarwani and Varshni [4] through an appropriate series expansion of the solution of the Schrödinger equation. Although the latter method is most interesting and yields remarkably accurate results, it seems to be restricted to the ground state of the SSC potential.

Recently, Ixaru *et al* [6] have proposed a method for integrating the Schrödinger equation based on the propagation matrix. This procedure has been simplified by Fernández *et al* [7] to treat quantum-mechanical models with potentials that can be expanded in a Taylor series about every point in a grid. The purpose of this paper is to show that the matrix propagation method and the power series expansion are suitable for calculating critical screening parameters. We develop the method in section 2 and discuss results for the SSC amd ECSC potentials in section 3.

* Work partly supported by Fundación Antorchas, Project No. 11089/1.

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0305-4470/91/092051+08$03.50

2. The matrix propagation method

We consider the Sturm–Liouville equation

$$P(x)Y''(x)+Q(x)Y'(x)+R(E,x)Y(x)=0 \qquad a<x<b \tag{2a}$$

where R depends parametrically on the eigenvalue E and $Y(x)$ satisfies the boundary conditions

$$\alpha_1 Y(a)+\alpha_2 Y'(a)=0 \qquad \beta_1 Y(b)+\beta_2 Y'(b)=0. \tag{2b}$$

It is further assumed that the functions $Q(x)/P(x)$ and $R(E,x)/P(x)$ do not have singular points in (a, b). The values of the parameter E for which the boundary conditions $(2b)$ are satisfied are the eigenvalues of the Sturm–Liouville problem.

For the sake of simplicity we define

$$\Phi(x)=\begin{pmatrix} Y(x) \\ Y'(x) \end{pmatrix} \tag{3}$$

so that the Sturm–Liouville equation can be more conveniently rewritten in matrix form:

$$P(x)\Phi'(x)=Z(x)\Phi(x) \tag{4a}$$

where

$$Z(x)=\begin{pmatrix} 0 & P(x) \\ -R(x) & -Q(x) \end{pmatrix}. \tag{4b}$$

We further define a 2×2 propagation matrix $T(x, y)$ so that the solution at any point $a\leqslant x\leqslant b$ is obtained from the solution at any other point, say $a\leqslant y\leqslant b$, according to

$$\Phi(x)=T(x,y)\Phi(y). \tag{5a}$$

In order to satisfy this equation for $x=y$ it is necessary that

$$T(y,y)=I \tag{5b}$$

is the identity matrix. On differentiating equation $(5a)$ with respect to x and using equations (4), it follows that $T(x, y)$ is a solution of

$$P(x)T'(x,y)=Z(x)T(x,y) \tag{6}$$

with the boundary condition $(5b)$. From now on the prime denotes differentiation with respect to the first argument.

It is not difficult to see that the propagation matrix can be written

$$T(x,y)=\begin{pmatrix} A(x,y) & B(x,y) \\ A'(x,y) & B'(x,y) \end{pmatrix} \tag{7}$$

where $A(x, y)$ and $B(x, y)$ are two linearly independent solutions of equation $(2a)$ satisfying

$$A(y,y)=B'(y,y)=1 \qquad A'(y,y)=B(y,y)=0. \tag{8}$$

Therefore, it is sufficient to obtain one element of each column of T. Furthermore, if for a given x_0, $a<x_0<b$, we know both $A(x, x_0)$ and $B(x, x_0)$ then we can write a solution of equation $(2a)$ and its derivative in terms of E, $Y(x_0)$ and $Y'(x_0)$:

$$Y(x)=Y(x_0)A(x,x_0)+Y'(x_0)B(x,x_0) \tag{9a}$$

$$Y'(x)=Y(x_0)A'(x,x_0)+Y'(x_0)B'(x,x_0). \tag{9b}$$

On introducing these equations into equations (2*b*) we obtain a system of two linear homogeneous equations with two unknowns, namely, $Y(x_0)$ and $Y'(x_0)$. Therefore, in order to have solutions other than the trivial one the determinant of the system has to vanish, leading to

$$\begin{aligned}\alpha_1\beta_1(A(a,x_0)B(b,x_0)-A(b,x_0)B(a,x_0))\\ +\alpha_1\beta_2(B(a,x_0)A'(b,x_0)-A(a,x_0)B'(b,x_0))\\ +\alpha_2\beta_2(A(b,x_0)B'(a,x_0)-A'(a,x_0)B(b,x_0))\\ +\alpha_2\beta_2(A'(a,x_0)B'(b,x_0)-A'(b,x_0)B'(a,x_0))=0\end{aligned} \tag{10}$$

the roots of which are the eigenvalues of the Sturm–Liouville equation. For each eigenvalue we also obtain the ratio $Y'(x_0)/Y(x_0)$, which determines the eigenfunction completely but for a normalization factor.

For a small enough h value, it is often possible to obtain accurate approximations to $A(x+h,x)$ and $B(x+h,x)$ for every x value so that $\Phi(x+h)=T(x+h,x)\Phi(x)$ according to equation (5*a*). This fact enables one to build a grid $x_0, x_{-1}, \ldots, x_{-m}=a$, $x_1, x_2, \ldots, x_n=b$, where $x_j=x_0+jh$, and calculate

$$T(a,x_0)=\prod_{j=1}^{m} T(x_{-j},x_{1-j}) \tag{11a}$$

$$T(b,x_0)=\prod_{j=1}^{n} T(x_j,x_{j-1}). \tag{11b}$$

Equations (11) give us $A(a,x_0)$, $A'(a,x_0)$, $A(b,x_0)$, $A'(b,x_0)$, $B(a,x_0)$, $B'(a,x_0)$, $B(b,x_0)$ and $B'(b,x_0)$ in terms of E, which are then introduced into equation (10) to obtain the eigenvalues.

Ixaru *et al* [6] proposed an interesting and powerful way of calculating the solutions $A(x,y)$ and $B(x,y)$. However, in some cases it is much easier to proceed, as shown by Fernández *et al* [7] for the simpler case of the Schrödinger equation. In what follows we generalize their results to the case of the Sturm–Liouville equation. If $Z(x+h)$ can be expanded in a Taylor series around $h=0$,

$$Z(x+h)=\sum_{j=0}^{\infty} Z^{(j)}(x)h^j \tag{12}$$

then $T(x+h,x)$ can also be expanded as

$$T(x+h,x)=\sum_{j=0}^{\infty} T^{(j)}(x,x)h^j \tag{13}$$

where $T^{(0)}(x,x)=T(x,x)=I$. The elements of the 2×2 matrices $T^{(j)}(x,x)$ are easily obtained by expandinng equation (4*a*) in a power series of h. In fact, if $P(x+h)=P(x)+P^{(1)}(x)h+\ldots$ we have the following recurrence relation for the 2×2 matrices $T^{(k)}$:

$$\begin{aligned}T^{(k+1)}(x,x)=[(k+1)P(x)]^{-1}\Bigg(\sum_{j=0}^{k} Z^{(j)}(x)T^{(k-j)}(x,x)\\ -\sum_{j=1}^{k}(k-j+1)P^{(j)}(x)T^{(k-j+1)}(x,x)\Bigg).\end{aligned} \tag{14}$$

In order to calculate the eigenvalues and eigenfunctions we proceed as follows. First, we obtain the Taylor coefficients $T^{(k)}$ from the recurrence relation (14) and construct an approximate propagation matrix by truncating the infinite series (13) up to a given order (say h^N). Notice that according to equation (7) we have to calculate only the first row of T. This step is straightforward provided the derivatives of $P(x)$, $Q(x)$ and $R(E, x)$ can be obtained explicitly. In this way we calculate $T(x_j, x_{j-1}) = T(x_{j-1}+h, x_{j-1})$, $j=1, 2, \ldots, n$ and $T(x_{-j}, x_{1-j}) = T(x_{1-j}-h, x_{1-j})$, $j=1, 2, \ldots, m$. Secondly, we obtain $T(a, x_0)$ and $T(b, x_0)$ through equations (11). According to equation (7) these matrices give us $A(x, x_0)$, $B(x, x_0)$, and their derivatives at a and b which are then substituted into equation (10) to obtain the eigenvalues. For a given eigenvalue the ratio $Y'(x_0)/Y(x_0)$, which according to equations (9) determines the eigenfunction and its first derivative, is also derived from the boundary conditions. As T, Z and the coefficients of their Taylor series are 2×2 matrices the computation of equations (11-14) offers no difficulty. If the matrix products are written explicitly and calculated progressively along the grid, it is not necessary to store these matrices in order to calculate the eigenvalues. If the eigenfunctions are required one has to store only $A((x_j, a)$, $A(x_j, b)$, $B(x_j, a)$, and $B(x_j, b)$ for the desired grid points.

3. Results and discussion

The radial part of the time-independent Schrödinger equation for a central-field model can be written as

$$F''(r)+[2(E-V(r))-l(l+1)/r^2]F(r)=0 \tag{15a}$$

where $l=0, 1, \ldots$ is the angular momentum quantum number and the solutions for $E<0$ satisfy

$$F(0)=F(\infty)=0. \tag{15b}$$

We specialize in the screened Coulomb potentials (1) and in the calculation of the critical parameters which, as said before, are those δ values for which the largest bound-state energy E equals zero. The boundary conditions in such cases are known to be [4] $F(0)=0$ and $F(\infty)=\text{constant}=1$.

In order to apply a shooting method to the time-independent Schrödinger equation for the ECSC potential, Singh and Varshni [5] proposed the change of variables $r=x/(1-x)$ so that the interval $0\leqslant r<\infty$ is mapped onto $0\leqslant x<1$. The advantage of this transformation is a remarkable decrease in the number of required grid points (compare, for instance, the calculation in [1] with the one discussed below). We find it more convenient to use the more general mapping

$$r=Kx/(1-x) \tag{16}$$

where K is an adjustable parameter. The Schrödinger equation (15a) can be rewritten in the new variable x as a Sturm-Liouville equation (2a) where

$$\begin{aligned} &P(x)=(1-x)^4 \qquad Q(x)=-2(1-x)^3 \\ &R(x)=2K^2[E-V(r(x)]-l(l+1)(l-x)^2/x^2 \end{aligned} \tag{17}$$

and $Y(x)=F(r(x))$.

The K value is set so that the coefficients of the Taylor series for $R(x+h)$ about $h=0$ change smoothly with δ. An appropriate choice is $K=1/\delta$, so that δ does not appear in the exponential.

The boundary conditions for the case $E=0$, namely $Y(0)=0$ and $Y(1)=1$, can be rewritten

$$Y(0)=0 \qquad Y'(1)=0 \tag{18}$$

which is a particular case of equation (2*b*) where $\alpha_2=\beta_1=0$, $\alpha_1=\beta_2=1$, $a=0$ and $b=1$. Therefore, the critical screening parameters can be obtained from the roots of

$$A(0, x_0)B'(1, x_0)-A'(1, x_0)B(0, x_0)=0. \tag{19}$$

in which E is set equal to zero.

When applying standard numerical integration algorithms to the eigenvalue equation (15), one has to substitute $F'(r_{max})=1$ for $F'(\infty)=1$ for a sufficiently large value of r_{max}. In the present case we replace the actual end points $a=0$ and $b=1$ in equation (19) by the approximate ones $a=h$ and $b=1-h$, respectively, so that the latter approach the former as $h\to 0$. Notice that with this choice $r_{max}=(1-h)/\delta h$ is a large number when h is small. The absolute value of $f(\delta)=A(h, x_0)B'(1-h, x_0)-A'(1-h, x_0)B(h, x_0)$ for $E=0$ is large when $\delta\neq\delta_c$. For this reason the critical screening parameters, i.e. the roots of $f(\delta)=0$, are sharply defined and accurate results can be easily obtained by means of the Newton–Raphson method. This algorithm can be implemented with either numerical or analytical derivatives $df(\delta)/d\delta$. In the latter case one exploits the fact that the recurrence relation (14) can be differentiated with respect to δ giving a recurrence relation for the derivatives of the matrix elements of T which enable one to obtain $df(\delta)/d\delta$.

The singularities at the end points $x=0$ and $x=1$ do not offer any difficulty because the solutions of the Sturm–Liouville equation, which have to satisfy the boundary conditions (18), cannot be singular at such points, otherwise one would not find any root of $f(\delta)=0$.

We have calculated the critical screening parameters δ_c using a truncated propagation matrix,

$$T(x+h, x)=\sum_{j=0}^{N} T^{(j)}(x, x)h^j \tag{20}$$

for several values of h and N. The convergence of the method is illustrated in table 1 for the ground state of the ECSC. We choose this state because as it has the largest δ_c value it is the most difficult to treat, and this model because Singh and Varshni [5] obtained accurate critical parameters by means of a shooting method.

Table 1 shows that the method converges quickly and smoothly and that the convergence velocity is larger the larger the value of N. Since the same limit is obtained with different values of N and h (both decreasing h and/or increasing N result in increasing the number of operations) we may conclude that the accumulation of round-off errors do not affect the figures considered.

We also calculated the critical screening parameters using the Numerov method described by Leroy and Wallace [8]. Because of the form of the ground-state eigenfunction of the Sturm–Liouville equation treated here we were unable to implement the matching of the inward and outward integrations at an intermediate point proposed by those authors [8]. For this reason, we integrated the Sturm–Liouville equation from 1 to 0 (strictly speaking from $1-h$ to h). Besides, we used a Numerov algorithm of order h^2 because we found it difficult to improve its accuracy for the problem discussed here. It is clear from table 1 that the Numerov procedure is comparable to the matrix propagation method of order h^2 which converges too slowly to obtain highly accurate

Table 1. Convergence of the algorithm for the state 1s of the ECSC.

h	Numerov (h^2)	Present ($N=2$)	Present ($N=4$)
$\frac{1}{10}$	0.723 258 945 359 290	0.744 702 036 214 895	0.720 368 879 064 621
$\frac{1}{20}$	0.721 280 418 220 135	0.725 825 101 270 036	0.720 408 077 612 956
$\frac{1}{40}$	0.720 704 785 383 642	0.721 751 365 663 931	0.720 525 091 385 301
$\frac{1}{80}$	0.720 569 338 729 548	0.720 819 816 375 769	0.720 524 027 777 208
$\frac{1}{160}$	0.720 535 395 818 925	0.720 596 524 725 727	0.720 524 082 333 809
$\frac{1}{320}$	0.720 526 913 164 771	0.720 542 002 163 625	0.720 524 085 654 350
$\frac{1}{740}$	0.720 524 792 690 076	0.720 528 540 294 929	0.720 524 085 867 547
$\frac{1}{1480}$	0.720 524 262 583 198	0.720 525 196 369 880	0.720 524 085 881 047
$\frac{1}{2960}$	0.720 524 130 057 215	0.720 524 363 112 254	0.720 524 085 881 896
$\frac{1}{5920}$	0.720 524 096 925 766	0.720 524 155 140 414	0.720 524 085 881 950
h	Present ($N=6$)	Present ($N=8$)	Present ($N=10$)
$\frac{1}{10}$	0.720 550 260 489 451	0.720 588 488 150 313	0.720 457 583 278 684
$\frac{1}{20}$	0.720 522 169 569 028	0.720 524 925 980 976	0.720 523 879 880 154
$\frac{1}{40}$	0.720 524 088 600 926	0.720 524 085 325 165	0.720 524 085 813 419
$\frac{1}{80}$	0.720 524 085 883 120	0.720 524 085 881 310	0.720 524 085 882 200
$\frac{1}{160}$	0.720 524 085 881 958	0.720 524 085 881 953	0.720 524 085 881 953
$\frac{1}{320}$	0.720 524 085 881 953	0.720 524 085 881 953	
$\frac{1}{740}$	0.720 524 085 881 953		
h	Present ($N=12$)	Present ($N=14$)	Present ($N=16$)
$\frac{1}{10}$	0.720 569 545 846 230	0.720 281 084 700 952	0.721 730 061 765 772
$\frac{1}{20}$	0.720 524 361 079 354	0.720 523 547 432 746	0.720 524 664 082 543
$\frac{1}{40}$	0.720 524 085 862 167	0.720 524 085 925 071	0.720 524 085 865 420
$\frac{1}{80}$	0.720 524 085 881 890	0.720 524 085 881 964	0.720 524 085 881 952
$\frac{1}{160}$	0.720 524 085 881 953	0.720 524 085 881 953	0.720 524 085 881 953

critical screening parameters. In our opinion the algorithm proposed here can be improved more easily and systematically than other numerical approaches. To do this, one simply includes more terms in equation (20), which are easily obtained recursively from equation (14), and decreases h.

As shown in table 1, the use of approximate end points is not a serious limitation to the accuracy of the method, provided h is sufficiently small. However, since the actual boundary conditions are recovered only when $h \to 0$ it is useless to increase N indefinitely without decreasing h. On the other hand, one can in principle obtain the exact answer when $h \to 0$, disregarding the value of N ($N > 0$) used. In practice, however, it is not advisable to use a too-small N value because it may result in a too-slow convergence. Because the optimum choice of N for a given problem is difficult to estimate beforehand we resorted to numerical experiment. We computed the time required to propagate the solution from 0 to 1 for different choices on N and h leading to the same accuracy (as a test example we used the value $\delta_c^{\mathrm{ECSC}}(1s) = 0.720\,524\,085\,881\,95$). As the fastest case is $N=6$ and $h=\frac{1}{160}$, we choose this value of N to calculate all the screening parameters shown in tables 2 and 3. These results exhibit the digits that are stable when h is halved. More accurate screening parameters can in principle be obtained by means of a convergence-accelerating procedure such as Richardson extrapolation, but we deem such improvement unnecessary.

The method proposed here is simple and powerful. Among its advantages we mention that one can improve the accuracy of the algorithm easily and systematically.

Table 2. Critical screening parameters of the ECSC potential calculated by means of the present algorithm with accuracy h^6.

	1s		
$h=\frac{1}{640}$	0.720 524 085 881 953		
[5]	0.720 524 085 88		
	2s	2p	
$h=\frac{1}{640}$	0.166 617 599 995 557		
$h=\frac{1}{1280}$		0.148 205 032 643	
[5]	0.166 617 60	0.148 205 03	
	3s	3p	3d
$h=\frac{1}{640}$	0.072 436 991 196 400		
$h=\frac{1}{1280}$		0.068 712 143 689	0.063 581 546 150 8
[5]	0.072 436 99	0.068 712 14	0.063 581 54
	4s	4p	4d
$h=\frac{1}{640}$	0.040 427 221 157 776		
$h=\frac{1}{1280}$		0.03 926 340 117 92	0.037 405 048 313 45
[5]	0.040 427 22	0.03 926 340	0.037 405 05
	5s	5p	5d
$h=\frac{1}{640}$	0.025 787 301 102 823		
$h=\frac{1}{1280}$		0.025 315 625 317 70	0.024 500 014 162 25
[5]	0.025 787 30	0.025 315 62	0.024 500 01
	6s	6p	6d
$h=\frac{1}{640}$	0.017 878 285 415 406		
$h=\frac{1}{1280}$		0.017 652 070 207 41	0.017 242 903 688 98
[5]	0.017 878 28	0.017 652 07	0.017 242 90
	4f		
$h=\frac{1}{640}$	0.035 241 242 180 742		
[5]	0.035 241 24		
	5f	5g	
$h=\frac{1}{1280}$	0.023 482 156 409 613	0.022 371 423 947 612	
[5]	0.023 482 16	0.022 371 42	
	6f	6g	6h
$h=\frac{1}{640}$			0.015 455 476 970 671
$h=\frac{1}{1280}$	0.016 708 150 087 85	0.016 099 483 083 173	
[5]	0.016 708 15	0.016 099 48	0.015 455 48

In fact, when the matrix $Z(x+h)$ can be expanded in a power series of h the corrections are quickly calculated by means of simple recurrence relations (cf. equation (14)). All the results shown here were obtained by means of a personal computer and an algorithm written in Pascal. The accuracy of the method can be seen in that our double-precision results appear to be more accurate than the ones obtained by Singh and Varshni [5] using quadruple precision. The calculations reported in this paper constitute a wholly demanding test for any numerical integration method because the most difficult state to treat is the one with energy close to zero.

The main disadvantage of our approach is that it is not so easily applied when the matrix Z cannot be expanded in a Taylor series. However, in such a case one may approximate the matrix elements of Z by means of polynomials or other kinds of approximants. Furthermore, the powerful perturbation method proposed by Ixaru [6] is also available.

Table 3. Critical screening parameters of the SSC potential calculated by means of the present algorithm with accuracy h^6.

	1s		
$h=\frac{1}{640}$	1.190 612 421 060 618		
[1]	1.190 6		
	2s	2p	
$h=\frac{1}{320}$	0.310 209 282 713 937		
$h=\frac{1}{1280}$		0.220 216 806 61	
[1]	0.310 1	0.220 1	
	3s	3p	3d
$h=\frac{1}{640}$	0.139 450 294 064 18		0.091 345 120 771 732
$h=\frac{1}{1280}$		0.112 710 498 36	
[1]	0.139 5	0.112 7	0.091 3
	4s	4p	4d
$h=\frac{1}{640}$	0.078 828 110 273 172		0.058 105 052 754 469
$h=\frac{1}{1280}$		0.067 885 376 10	
[1]	0.078 8	0.067 9	0.058 1
	5s	5p	5d
$h=\frac{1}{640}$	0.050 583 170 560		0.040 024 353 938 325
$h=\frac{1}{1280}$		0.045 186 248	
[1]	0.050 6	0.045 2	0.040 0
	5f		
$h=\frac{1}{320}$	0.049 831 132 318 646		
[1]	0.049 8		
	6f		
$h=\frac{1}{640}$	0.035 389 389 799 949		
[1]	0.035 4		

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