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Variational trial functions in quantum theory II. Continuous spectrum

T L JOHN† and K L WILLIAMS‡

† Department of Applied Mathematics and Mathematical Physics, University College, Cardiff, UK

‡ Computing Centre, University College, Cardiff, UK

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Abstract. A method given in the previous paper for the calculation of variational trial functions is applied to the continuous spectra of some simple one and two particle systems.

1. Introduction

In a previous paper (John and Williams 1972, referred to as I) we presented a method for determining variational trial functions and applied them to the calculation of the ground state of one and two particle systems. In the present paper, we describe applications of these trial functions to the continuous spectrum of similar systems. We also discuss and compare this method with the variation–iteration methods of McEachran *et al* (1965) and Kraidy and Fraser (1966). As the main purpose of the paper is to discuss and assess the usefulness of the method, all applications are restricted to simple systems and approximations where exact solutions are readily available in the literature; thus no new results are presented.

2. Trial functions for one particle systems

As described in I, trial functions for a particle of momentum k and orbital angular momentum l scattered by the central field potential $U(r)$, where $rU(r) \to 0$ as $r \to \infty$, are defined as follows:

type 1

$$f_l^1(k^2|r) = \frac{N^1}{k} \cos \eta_l^1 j_l(kr) - \int_0^\infty G_l(k^2|x, r)U(x)\phi(x)\,dx \tag{1}$$

type 2 (iterated functions)

$$f_l^{(n)1}(k^2|r) = \frac{N^{(n)1}}{k} \cos \eta_l^1 j_l(kr) - \int_0^\infty G_l(k^2|x, r)U(x) f_l^{(n-1)1}(k^2|x)\,dx \qquad n \geqslant 1 \tag{2}$$

where η_l^t is the phase shift parameter and N a normalizing factor†, which will be defined later. The free electron Green function is given by

$$\begin{aligned} G_l(k^2|x,r) &= \frac{1}{k}\mathrm{j}_l(kx)\mathrm{n}_l(kr) \qquad 0 \leqslant x \leqslant r \\ &= \frac{1}{k}\mathrm{j}_l(kr)\mathrm{n}_l(kx) \qquad r < x < \infty \end{aligned} \tag{3}$$

and the functions $\mathrm{j}_l(x)$ and $\mathrm{n}_l(x)$ can be expressed in terms of the Bessel functions

$$\begin{aligned} \mathrm{j}_l(x) &= (\tfrac{1}{2}\pi x)^{1/2}\mathrm{J}_{l+\frac{1}{2}}(x) \\ \mathrm{n}_l(x) &= (-1)^l(\tfrac{1}{2}\pi x)^{1/2}\mathrm{J}_{-l-\frac{1}{2}}(x). \end{aligned} \tag{4}$$

The functions $\phi(x)$ and $f_l^{(0)t}(k^2|x)$ will in general depend on a set of parameters c_i $(i = 1, \ldots, m)$. In most applications, the trial functions are usually taken to be linear functions of the parameters so that computations are reduced to evaluating the appropriate variational integrals and solving sets of simultaneous equations. The general form for ϕ or $f_l^{(0)t}$ we shall take to be

$$\left.\begin{matrix} \phi(x) \\ f_l^{(0)t}(k^2|x) \end{matrix}\right\} = u_0(x) + \sum_{i=1}^{m} c_i u_i(x). \tag{5}$$

These trial functions are suitable for applications in Schwinger's method (see Blatt and Jackson 1949) and Hulthén–Kohn methods. The Hulthén–Kohn methods can be classified according to the normalizing factor N^t, for $N^t = \sec\eta_l^t$, we have 'tangent' methods, for example, the methods of Kohn (1948), Hulthén (1944) 1st method and Malik (1962), and for $N^t = k\,\mathrm{cosec}\,\eta_l^t$ we have 'cotangent' methods, for example, the 2nd method of Hulthén (1948). For a recent account of these and alternative methods see John (1967).

For 'tangent' methods, using ϕ defined by equation (5) the trial functions have the asymptotic forms

$$f_l^t(k^2|r) \underset{r\to\infty}{\sim} \frac{1}{k}\mathrm{j}_l(kr) + \left(\alpha_0 + \sum_{i=1}^{m} c_i\alpha_i\right)\mathrm{n}_l(kr) \tag{6}$$

where

$$\alpha_i = -\frac{1}{k}\int_0^\infty U(x)\mathrm{j}_l(kx)u_i(x)\,\mathrm{d}x \qquad i = 0, 1, \ldots, m. \tag{7}$$

Substituting $f_l^t(k^2|r)$ into the variational integral

$$L = \int_0^\infty f_l^t(k^2|r)\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{l(l+1)}{r^2} - U(r) + k^2\right) f_l^t(k^2|r)\,\mathrm{d}r \tag{8}$$

gives the condition

$$\delta\left(L + \alpha_0 + \sum_{i=1}^{m} c_i\alpha_i\right) = 0. \tag{9}$$

† This choice of normalization factor N enables calculations of the scattering length to be made by taking the limit $k \to 0$.

Following John (1967), we have alternative methods of solution depending on the choice of m of the $m+2$ equations used to calculate the parameters

$$L = 0$$

$$\frac{\partial L}{\partial c_i} = -\alpha_i \qquad i = 1, \ldots, m \tag{10}$$

$$\alpha_0 + \sum_{i=1}^{m} c_i \alpha_i = -\frac{1}{k} \int_0^\infty U(x) \mathrm{j}_l(kx) f_l^{\mathrm{I}}(k^2|x)\, \mathrm{d}x$$

and

$$\frac{1}{k} \tan \eta_l = \alpha_0 + \sum_{i=1}^{m} c_i \alpha_i + L \tag{11}$$

to calculate the phase shift.

The results for iterated type 2 functions with $n = 1$ are identical to those given by type 1. For $n \neq 1, f_l^{(n-1)\mathrm{I}}$ appearing in the integral part of equation (2) is of the form

$$f_l^{(n-1)\mathrm{I}}(k^2|x) = u_0^{(n-1)}(x) + \sum_{i=1}^{m} c_i u_i^{(n-1)}(x) \tag{12}$$

and the equivalent expression to (9) is

$$\delta\left(L + \alpha_0^{(n-1)} + \sum_{i=1}^{m} c_i \alpha_i^{(n-1)} \right) = 0 \tag{13}$$

where

$$\alpha_i^{(n)} = -\frac{1}{k} \int_0^\infty U(x) \mathrm{j}_l(kx) u_i^{(n)}(x)\, \mathrm{d}x \qquad i = 0, 1, \ldots, m. \tag{14}$$

The functions $u_i^{(n)}$ can be obtained from the recurrence relation

$$u_i^{(n)}(r) = \frac{1}{k} \mathrm{j}_l(kr) \delta_{i,0} - \int_0^\infty G_l(k^2|x, r) U(x) u_i^{(n-1)}(x)\, \mathrm{d}x \qquad n \geqslant 1 \tag{15}$$

$$u_i^{(0)}(x) = u_i(x).$$

The equations corresponding to (10) and (11) in this case are

$$L = 0$$

$$\frac{\partial L}{\partial c_i} = -\alpha_i^{(n-1)} \qquad i = 1, \ldots, m$$

$$\alpha_0^{(n-1)} + \sum_{i=1}^{m} c_i \alpha_i^{(n-1)} = -\frac{1}{k} \int_0^\infty U(r) \mathrm{j}_l(kr) f_l^{(n-1)\mathrm{I}}(k^2|\mathrm{r})\, \mathrm{d}r \tag{16}$$

and

$$\frac{1}{k} \tan \eta_l = \alpha_0^{(n-1)} + \sum_{i=1}^{m} c_i \alpha_i^{(n-1)} + L. \tag{17}$$

The asymptotic form of type 1 trial functions for 'cotangent' methods is

$$f_l^{\mathrm{I}}(k^2|r) \underset{r \to \infty}{\sim} \cot \eta_l^{\mathrm{I}} \mathrm{j}_l(kr) + \left(\alpha_0 + \sum_{i=1}^{m} c_i \alpha_i \right) n_l(kr) \tag{18}$$

thus it is necessary to impose the condition

$$\alpha_0 + \sum_{i=1}^{m} c_i \alpha_i = 1 \tag{19}$$

on the parameters in order to satisfy the boundary condition. We shall assume that c_m can be expressed in terms of the other c thus f_l^1 will now depend on the m parameters $(\cot \eta_l^1, c_1, \ldots, c_{m-1})$. The variational condition in this case is

$$\delta(L - k \cot \eta_l^1) = 0 \tag{20}$$

giving rise to alternative methods by choosing m of the $m+2$ equations

$$\begin{aligned} &L = 0 \\ &\frac{\partial L}{\partial (k \cot \eta_l^1)} = 1 \\ &\frac{\partial L}{\partial c_i} = 0 \qquad i = 1, \ldots, m-1 \\ &-1 = \frac{1}{k} \int_0^\infty U(x) j_l(kx) f_l^1(k^2|x)\, dx. \end{aligned} \tag{21}$$

The equation

$$k \cot \eta_l = k \cot \eta_l^1 + L \tag{22}$$

defines the phase shift.

3. The variation–iteration method

The variation–iteration method of McEachran *et al* and Kraidy and Fraser bears some similarity to the method discussed here. In the variation–iteration method, a set of functions $\mathscr{F}_l^{(n)}(k^2|r)$ is obtained from the integral equation

$$\mathscr{F}_l^{(n)}(k^2|r) = \frac{N^{(n)}}{k} \cos \eta_l^{(n)} j_l(kr) - \int_0^\infty G_l(k^2|x, r) U(x) \mathscr{F}_l^{(n-1)}(k^2|r)\, dr \qquad n \geqslant 1 \tag{23}$$

where

$$\begin{aligned} &N^{(n)} = \sec \eta_l^{(n)} \\ &\mathscr{F}_l^{(0)}(k^2|r) = \frac{1}{k} j_l(kr) \end{aligned} \tag{24}$$

for 'tangent' methods, and

$$\begin{aligned} &N^{(n)} = k \operatorname{cosec} \eta_l^{(n)} \\ &\mathscr{F}_l^{(0)}(k^2|r) = \cot \eta_l^{(0)} j_l(kr) + (1 - e^{-r})^{2l+1} \eta_l(kr) \end{aligned} \tag{25}$$

for 'cotangent methods'. $\eta_l^{(n)}$ is given by

$$\begin{aligned} \frac{1}{k} \int_0^\infty U(x) j_l(kx) \mathscr{F}_l^{(n)}(k^2|x)\, dx &= -\tan \eta_l^{(n)} \text{ (tangent methods)} \\ &= -1 \text{ (cotangent methods).} \end{aligned} \tag{26}$$

One parameter trial functions are defined as follows

$$\begin{aligned} f_l^1(k^2|r) &= p\mathscr{F}_l^{(n)}(k^2|r)+(1-p)\mathscr{F}_l^{(n-1)}(k^2|r) \\ f_l^1(k^2|r) &= q\mathscr{F}_l^{(n)}(k^2|r)+(1-q)\mathscr{F}_l^{(1)}(k^2|r) \end{aligned} \tag{27}$$

where p and q are parameters calculated by the equations

$$\frac{\partial L}{\partial p} = 0 \qquad \text{or} \qquad \frac{\partial L}{\partial q} = 0 \tag{28}$$

and the phase shift by

$$\tan \eta_l = \tan \eta_l^{(n)} + kL$$

or

$$k \cot \eta_l = k \cot \eta_l^{(n)} - L. \tag{29}$$

In applications these methods were compared with the Born iteration procedure, that is, solving equation (23) using equations (24) and a similar procedure with the cotangent normalization. The variation–iteration method in this context can be thought of as a way of speeding up the convergence of the Born method. However, there are certain drawbacks; firstly convergence is not always possible and secondly the computations involved in the iterations can be considerable especially when a large number of iterations are needed. In calculating the phase shifts for the elastic scattering of electrons by hydrogen atoms, when convergence was possible, it took from 3 to 16 iterations depending on the approximation for the wavefunction, the normalization, energy, spin and orbital angular momentum.

4. Applications to simple potentials

To illustrate the method described in § 2 we have chosen the cases of the scattering lengths† A_0 for the exponential potential

$$U(r) = -U_0 \exp\left(-\frac{r}{r_0}\right) \tag{30}$$

and the square well potential

$$\begin{aligned} U(r) &= -U_0 \qquad 0 \leqslant r \leqslant r_0 \\ &= 0 \qquad r > r_0 \end{aligned} \tag{31}$$

and the s wave phase shift for the square well potential (31). If we make a change of variable $r' = r/r_0$ and define $U_0' = U_0 r_0^2$, then all cases, exact and variational are covered taking $r_0 = 1$ and $U_0 = U_0'$.

† Note for the scattering length we have the limiting cases $j_0(kr)/k \to r$, $n_0(kr) \to 1$, $\eta_0^1/k \to A_0^1$ and

$$\begin{aligned} G_0(k^2|x,r) &\to x \qquad (0 \leqslant x \leqslant r) \\ &\to r \qquad (r < x < \infty) \end{aligned}$$

as $k \to 0$.

For the exponential potential the scaled scattering length A_0/r_0 is given by

$$\frac{A_0}{r_0} = \frac{\pi Y_0(2x_0)}{J_0(2x_0)} - 2(\gamma + \ln x_0) \tag{32}$$

where $x_0 = r_0(U_0)^{1/2}$, γ is Euler's constant ($\gamma = 0{\cdot}5772\ldots$) and $J_0(x)$ and $Y_0(x)$ are zero order Bessel functions. For the square well potential the scaled scattering length is given by the well known formula

$$\frac{A_0}{r_0} = \frac{\tan x_0}{x_0} - 1. \tag{33}$$

For the scattering length calculations, we have chosen ϕ and $f_0^{(0)\mathrm{I}}$ as follows

one parameter

$$\left.\begin{matrix}\phi(x) \\ f_0^{(0)\mathrm{I}}(0|x)\end{matrix}\right\} = c_1 x \tag{34}$$

two parameter

$$\left.\begin{matrix}\phi(x) \\ f_0^{(0)\mathrm{I}}(0|x)\end{matrix}\right\} \begin{matrix} = c_1 x & (0 \leqslant x \leqslant r) \\ = c_2 x & (r < x < \infty). \end{matrix} \tag{35}$$

For type 2 functions, calculations were restricted to one parameter functions and one iteration, that is, the function $f_0^{(1)\mathrm{I}}(0|r)$. The results for the exponential potential are given in table 1; they are in good agreement with the exact solution.

For the square well potential, because of the boundary conditions the wavefunction has to satisfy at $r = r_0$, $c_2 = c_1$, that is, (35) becomes identical to (34). Results using this function and a two parameter type 1 trial function with ϕ defined by

$$\phi(x) = c_1 x + c_2 x^2 \tag{36}$$

are given in table 2.

The s wave phase shift for the square well potential is given by the equation

$$\frac{\tan(kr_0 + \eta_0)}{kr_0} = \frac{\tan K}{K} \tag{37}$$

where $K^2 = r_0^2(U_0 + k^2)$. If we make K a constant we can cover all cases by varying kr_0. We can judge the accuracy of any approximate solution by the deviation of the left hand side of equation (37) from a constant value. The corresponding type 1 trial function in this case is defined by

$$\phi(x) = c_1 \sin kx. \tag{38}$$

The variational values of $\tan(kr_0 + \eta_0)/kr_0$ are given in table 3 for a number of values of K; these hardly deviate from a constant value. For $K = 2{\cdot}5$ the Kohn method yields a singular behaviour because the coefficient of one of the terms in the variational integral L is zero.

Table 1. Scaled scattering length A_0/r_0 for exponential potential

		One parameter							Two parameters				
	Trial function	Type 1†				Type 2†			Type 1‡				
x_0^2	Numerical	Hulthén 1	Hulthén 2	Kohn	Schwinger	Hulthén 1	Hulthén 2	Kohn	Hulthén 1	Hulthén 2	Kohn	Method 1§	Method 2§
0·20	0·458	0·458	0·458	0·458	0·458	0·458	0·458	0·458	0·458	0·458	0·458	0·458	0·458
0·50	1·475	1·474	1·473	1·474	1·475	1·475	1·475	1·475	1·475	1·475	1·475	1·475	1·475
0·80	3·375	3·355	3·351	3·359	3·375	3·375	3·375	3·375	3·374	3·374	3·375	3·374	3·374
1·00	6·007	5·911	5·888	5·924	6·004	6·006	6·005	6·006	6·005	6·004	6·005	6·004	6·004
2·25	−6·518	−7·040	−7·693	−7·365	−6·585	−6·559	−6·622	−6·582	−6·494	−6·564	−6·554	−6·551	−6·572
2·50	−5·322	−5·611	−6·385	−6·102	−5·395	−5·359	−5·441	−5·396	Complex	−5·370	−5·360	−5·357	−5·378
3·00	−3·960	Complex	−5·031	−4·771	−4·059	−3·968	−4·139	−4·072	−4·053	−4·023	−4·011	−4·009	−4·032
3·50	−3·102	Complex	−4·321	−4·054	−3·251	Complex	−3·388	−3·283	−3·217	−3·196	−3·179	−3·179	−3·206
4·00	−2·407	Complex	−3·874	−3·588	−2·639	Complex	−2·863	−2·703	−2·573	−2·553	−2·529	−2·532	−2·566

† Calculated with $\phi(x) = c_1 x$.

‡ Calculated with $\phi(x) = c_1 x \qquad 0 \leqslant x \leqslant r, \phi(x) = c_2 x \qquad r < x < \infty$.

§ These methods are described by John (1967).

Table 2. Scaled scattering length A_0/r_0 for square well potential

		One parameter							Two parameters				
	Trial function	Type 1†				Type 2†			Type 1‡				
x_0	Numerical	Hulthén 1	Hulthén 2	Kohn	Schwinger	Hulthén 1	Hulthén 2	Kohn	Hulthén 1	Hulthén 2	Kohn	Method 1§	Method 2§
1·00	0·557	0·557	0·557	0·557	0·557	0·557	0·557	0·557	0·557	0·557	0·557	0·557	0·557
1·30	1·771	1·769	1·768	1·769	1·771	1·771	1·771	1·771	1·771	1·771	1·771	1·771	1·771
1·50	8·401	8·309	8·300	8·310	8·400	8·400	8·400	8·400	8·400	8·400	8·400	Complex	8·400
1·75	−4·155	−4·198	−4·203	−4·199	−4·155	−4·155	−4·156	−4·155	−4·155	−4·155	−4·155	−4·155	−4·155
2·40	−1·382	−1·400	−1·404	−1·403	−1·382	−1.383	−1·383	−1·383	−1·382	−1·382	−1·382	−1·382	−1·382
3·00	−1·048	−1·075	−1·089	−1·086	−1·050	−1·051	−1·055	−1·054	−1·048	−1·048	−1·048	−1·048	−1·048
3·50	−0·893	Complex	−0·976	−0·971	−0·902	−0·890	−0·919	−0·916	−0·893	−0·893	−0·893	−0·893	−0·893
4·00	−0·711	Complex	−0·906	−0·900	−0·752	Complex	−0·815	−0·807	−0·713	−0·712	−0·712	−0·713	−0·713

† Calculated with $\phi(x) = c_1 x$.
‡ Calculated with $\phi(x) = c_1 x + c_2 x^2$.
§ These methods are described by John (1967).

Table 3. $\tan(kr_0+\eta_0)/kr_0$ for the square well potential calculated with type 1 trial functions and $\phi(x) = c_1 \sin kx$. H1 Hulthén's 1st method; H2 Hulthén's 2nd method; KN Kohn's method

K	0·1			1·0			1·4			2·5		
Exact	1·003			1·557			4·141			−0·299		
$U_0/(U_0+k^2)$	H1	H2	KN	H1	H2	KN	H1	H2	KN	H1	H2	KN
0·2							4·141	4·141	4·141	−0·299	−0·299	−0·299
0·3							—	—	—	−0·299	−0·299	−0·301
0·35							—	—	—	−0·299	−0·299	−0·305
0·3807							—	—	—	−0·300	−0·300	−3·868
0·3808		1·003†			1·557†		—	—	—	−0·300	−0·300	5·724
0·4							4·141	4·141	4·141	−0·300	−0·300	−0·287
0·6							4·140	4·140	4·140	−0·302	−0·303	−0·301
0·7							4·139	4·139	4·139	−0·305	−0·307	−0·304
0·8							4·137	4·137	4·137	−0·308	−0·311	−0·309
0·9							4·135	4·134	4·135	−0·312	−0·316	−0·314

† The variational methods for these cases give the same value to within an accuracy of 4 significant figures.

5. Electron–hydrogen exchange approximation scattering lengths

The equivalent integral equations to (1) and (2) for two electron systems, such as an electron in the field of a hydrogen atom, present a number of practical difficulties in calculations. As discussed in I, these difficulties are mainly due to the complicated expressions for the two particle Green functions. A way of avoiding these difficulties so that the wavefunction can be expressed in terms of one particle Green functions is to use the close coupling approximation for the wavefunction.

Adopting this method to calculate the scattering length for electron–hydrogen scattering in the exchange approximation (one of the simplest forms of the close coupling approximation) we have to solve the integro–differential equation

$$\left\{\frac{d^2}{dr^2}+2\left(1+\frac{1}{r}\right)e^{-2r}\right\}f^{\pm}(r) = \pm 2P(r)\left(-\tfrac{1}{2}\int_0^\infty P(x)f^{\pm}(x)\,dx + r^{-1}\int_0^r P(x)f^{\pm}(x)\,dx + \int_r^\infty P(x)f^{\pm}(x)x^{-1}\,dx\right) \quad (39)$$

where $P(x) = 2x\,e^{-x}$ and the + and − signs refer to the singlet and triplet wavefunctions.

The type 1 trial functions in this case are given by

$$f^{\pm 1}(r) = Nr + \int_0^\infty G_0(0|x,r)\left\{2\left(1+\frac{1}{x}\right)e^{-2x} \pm 2P(x)\left(-\tfrac{1}{2}\int_0^\infty P(x')\phi(x')\,dx' + x^{-1}\int_0^x P(x')\phi(x')\,dx' + \int_x^\infty P(x')\phi(x')x'^{-1}\,dx'\right)\right\}dx. \quad (40)$$

The iterated type 2 functions can be obtained by putting $\phi = f^{\pm 1}$ in the right hand side of equation (40). The scattering lengths are given in table 4, where ϕ is given by (34) and (35). Results for the central field approximation which takes no account of the electron spin are also included; this case corresponds to $P(x) = 0$ in equations (39) and (40). The

Table 4. Electron–hydrogen scattering lengths

Approximation			Central field	Exchange singlet case	Exchange triplet case
Trial function	Number of parameters	Method			
		Numerical	9·45	−8·10	−2·35
		Kohn	7·77	−8·26	−2·35
Type 1†	One	Hulthén 1	7·68	−8·25	−2·35
		Hulthén 2	7·25	−8·26	−2·35
		Schwinger	9·31	−8·17	−2·35
		Kohn	9·25	−8·25	−2·35
		Hulthén 1	9·24	−8·25	−2·35
Type 1‡	Two	Hulthén 2	9·21	−8·25	−2·35
		Method 1§	9.24	−8·25	−2·35
		Method 2§	9.18	−8·25	−2·32
		Kohn	9·31	−8·11	−2·35
Type 2†	One	Hulthén 1	9·31	−8·11	−2·35
		Hulthén 2	9·25	−8·11	−2·35

† $\phi(x) = c_1 x$.
‡ $\phi(x) = c_1 x \qquad 0 \leqslant x \leqslant r, \phi(x) = c_2 x \qquad r < x < \infty$.
§ These methods are described by John (1967).

one parameter calculations in the central field and symmetric case of the exchange approximation are not very accurate. There is some improvement using the two parameter functions, especially in the central field approximation. The iterated type 2 functions give the best results.

To improve accuracy we used

$$\phi(x) = c_1 x + c_2(1 - e^{-2x}). \tag{41}$$

We considered two cases, the two parameter function given by equation (41) and the one parameter function obtained by putting $c_1 = 1$ in equation (41); these results are given in table 5.

One of the most sensitive tests of trial functions for the particular cases considered here is the exchange approximation singlet case. This was illustrated in an earlier paper (John and Williams 1966), where the trial function

$$f^{+t}(r) = r + A_0^{+t}(1 - e^{-2r}) \tag{42}$$

applied in the Kohn, Hulthén 1 and Hulthén 2 methods gave the values $A_0^+ = -24$, $-1{\cdot}7$ (or $-16{\cdot}6$), 4·6 respectively. The results in tables 4 and 5 are in very much better agreement with the numerical value of $-8{\cdot}10$ obtained by Seaton (1957).

6. Conclusions

The method presented here together with the simple applications have shown it to be both useful and accurate. The iteration procedure used to calculate type 2 functions can involve considerable computations. Here, we have confined ourselves to very simple

Table 5. Electron–hydrogen scattering lengths

Approximation			Central field	Exchange singlet case	Exchange triplet case
Trial function	Number of parameters	Method			
		Numerical	9·45	−8·10	−2·35
Type 1†	One	Kohn	9·43	−8·59	—
		Hulthén 1	9·43	−8·53	—
		Hulthén 2	9·43	−8·68	—
		Schwinger	9·43	−8·03	−2·35
		Kohn	—	−8·11	−2·35
Type 1‡	Two	Hulthén 1	—	−8.10	−2·35
		Hulthén 2	—	−8·11	−2·35
		Method 1§	—	complex	−2.35
		Method 2§	—	complex	−2·35

† $\phi(x) = x + c_1 x^2$.
‡ $\phi(x) = c_1 x + c_2 x^2$.
§ These methods are described by John (1967).

functions so that the integrals can be worked out analytically. In cases when this is not possible then numerical techniques can be adopted. However, this can involve as much work as the numerical solution of the original Schrödinger equation, particularly when a large number of iterations are needed. Type 1 trial functions seem to have some advantage from the computational standpoint over type 2 functions, as it is easier to introduce an extra parameter in the trial function than an extra iteration, when improved accuracy is required.

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