Aust. J. Phys., 1988, **41**, 47–53

A Least Squares Computational Method for the Scattering Amplitude

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Abstract

A new least squares computational method for the scattering amplitude is proposed. This may be applied without difficulty to atomic and other scattering computations. The approach is expected to give converged results of high accuracy and also to be free from major numerical instabilities. As an example a numerical computation is carried out following the method and some results are presented in partial support of the claim.

1. Introduction

A computational method (see Das 1978, 1979; Das *et al.* 1981; Das and Biswas 1981) has been successfully applied in several electron–atom and positron–atom collision problems (see Das 1979, 1981; Das *et al.* 1981; Das and Biswas 1981; Das and Saha 1981, 1982; Das and Bhattacharyya 1983, and references therein). The method always leads to results of moderate accuracy for intermediate and high energies. There have been attempts to improve the method (see Das *et al.* 1982; Khare and Kusum Lata 1984; Khare and Satya Prakash 1985), but little success has been achieved so far. In the present work we propose a new computational method following a somewhat different path. This approach, for obvious reasons, is expected to give converged results of high accuracy. The method is, moreover, expected to be free from major numerical instabilities. We first describe the method in connection with a potential scattering problem, and then extend it to an electron–atom scattering problem.

2. New Computational Method

(a) Scattering by a Yukawa Potential

We first consider the computation of the scattering amplitude by the Yukawa potential

$$V(r) = g \exp(-\lambda r)/r .$$

Here the scattering state may be expanded in the form

$$|\psi_i^{(+)}\rangle = |k_i\rangle + \int d^3p \, \frac{a(q)}{E - E(q) + i\epsilon} |q\rangle , \qquad (1)$$

0004-9506/88/010047$03.00

where the expansion coefficient $a(q)$ is unknown and is to be determined. So that a least squares approach is applicable, we must first find some suitable set of basis functions for an expansion of $a(q)$, which is a function of q and θ only for a local central potential. Now for simple reasons well known basis functions such as the Laguerre functions for q and the Legendre polynomials for θ are unsuitable. We propose instead to use $1/\{(q-\mu_l k_i)^2+\lambda_m^2\}$, with a discrete set of values for the parameters λ_m and μ_l, as basis functions in the momentum space. These are nothing but the Fourier transform of $\exp(-\lambda_m r)\exp(i\mu_l k_i . r)/4\pi r$. It may be seen that a combination of these functions for different values of λ_m and μ_l is sufficient to represent a function of the form $\Sigma_n R_n^{(+)}(r) P_n(\cos\theta)$ in which $R_n^{(+)}(r) \sim r^n$ near the origin. Now a choice of the parameters λ_m is rather simple. As $1/\lambda$ is the range of the potential one may choose the set $\lambda, 2\lambda, 3\lambda$ etc. as values of λ_m. A good choice for the μ_l is not so obvious, but some values including the value one may be chosen for these. Thus, a trial scattering state may be taken as

$$|\psi_t^{(+)}\rangle = |k_i\rangle + \sum_{ml} C_{ml} \int d^3q \frac{|q\rangle}{\{E-E(q)+i\epsilon\}\{(q-\mu_l k_i)^2+\lambda_m^2\}}, \tag{2}$$

where C_{ml} are complex variational parameters.

Next we operate on equation (2) by $(E-H)$:

$$(E-H)|\psi_t^{(+)}\rangle = -V|k_i\rangle + \sum_{ml} C_{ml} \int d^3q\, |q\rangle \frac{1}{(q-\mu_l k_i)^2+\lambda_m^2}$$

$$- \sum_{ml} C_{ml} \int d^3q \frac{V|q\rangle}{\{E-E(q)+i\epsilon\}\{(q-\mu_l k_i)^2+\lambda_m^2\}}. \tag{3}$$

The states $|p\rangle$ for different p form a complete set. Thus equations for the C_{ml} may be obtained by taking the scalar product of equation (3) with $|p\rangle$ and putting the result equal to zero:

$$-\langle p|V|k_i\rangle + \sum_{ml} C_{ml} \frac{1}{(p-\mu_l k_i)^2+\lambda_m^2}$$

$$- \sum_{ml} C_{ml} \int d^3q \frac{\langle p|V|q\rangle}{\{E-E(q)+i\epsilon\}\{(q-\mu_l k_i)^2+\lambda_m^2\}} = 0. \tag{4}$$

These equations may be solved by the least squares method.

Thus, we write the equations as

$$\sum_{ml} C_{ml} F_{ml}(p) - Y(p) = 0,$$

and minimise

$$\int |\sum_{ml} C_{ml} F_{ml}(p) - Y(p)|^2 \, dp\, d\Omega_p.$$

The corresponding minimising equations are

$$\sum_{ml} \int dp\, d\Omega_p\, F^*_{m'l'}(p) F_{ml}(p) C_{ml} - \int dp\, d\Omega_p\, F^*_{m'l'}(p) Y(p) = 0, \tag{5}$$

for all pairs $(m'l')$. This gives the estimated values of C_{ml} which we denote by C^*_{ml}. Finally, the approximate T-matrix element is obtained from

$$T = \langle \boldsymbol{k}_f \,|\, V \,|\psi_t^{(+)}\rangle,$$

where $|\psi_t^{(+)}\rangle$ is given by equation (2) with C_{ml} replaced by the estimated values C^*_{ml}. Thus, we have

$$T = \langle \boldsymbol{k}_f|\, V|\, \boldsymbol{k}_i\rangle + \sum_{ml} C^*_{ml} \int \mathrm{d}^3 q \, \frac{\langle \boldsymbol{k}_f|\, V|\, \boldsymbol{q}\rangle}{\{E - E(q) + \mathrm{i}\epsilon\}\{(\boldsymbol{q} - \mu_l \boldsymbol{k}_i)^2 + \lambda_m^2\}}. \tag{6}$$

Next we illustrate the quality of the trial scattering state by considering its asymptotic behaviour. For this we have

$$\begin{aligned}
\psi_t^{(+)}(\boldsymbol{r}) &= \langle \boldsymbol{r}|\psi_t^{(+)}\rangle \\
&= \langle \boldsymbol{r}|\, \boldsymbol{k}_i\rangle + \sum_{ml} C_{ml} \int \mathrm{d}^3 q \, \frac{\langle \boldsymbol{r}|\, \boldsymbol{q}\rangle}{\{E - E(q) + \mathrm{i}\epsilon\}\{(\boldsymbol{q} - \mu_l \boldsymbol{k}_i)^2 + \lambda_m^2\}} \\
&= \frac{\exp(\mathrm{i}\boldsymbol{k}_i \cdot \boldsymbol{r})}{(2\pi)^{\frac{3}{2}}} + \sum_{ml} C_{ml} \int \mathrm{d}^3 q \, \exp(\mathrm{i}\boldsymbol{q} \cdot \boldsymbol{r}) \exp\{-\mathrm{i}(\boldsymbol{q} - \mu_l \boldsymbol{k}_i) \cdot \boldsymbol{r}'\} \\
&\quad \times \exp(-\lambda_m r')/(2\pi)^{\frac{3}{2}} 4\pi \{E - E(q) + \mathrm{i}\epsilon\} \\
&= \exp(\mathrm{i}\,\boldsymbol{k}_i \cdot \boldsymbol{r})/(2\pi)^{\frac{3}{2}} - \sum_{ml} C_{ml} \int \mathrm{d}^3 q \, \mathrm{d}^3 r' \, \exp(\mathrm{i}\,\boldsymbol{q} \cdot \boldsymbol{R}) \\
&\quad \times \exp\{\mathrm{i}\,\mu_l \boldsymbol{k}_i \cdot \boldsymbol{r}'\} \exp(-\lambda_m r')/(2\pi)^{\frac{5}{2}} (q^2 - k^2 - \mathrm{i}\epsilon) r'.
\end{aligned}$$

The q integration gives a factor $2\pi^2 \exp(\mathrm{i}\,kR)/R$, where $R = |\boldsymbol{r} - \boldsymbol{r}'|$. Thus for $r \to \infty$ we have $R \approx r - r' \cos\theta$, where θ is the angle between $\boldsymbol{r}$ and $\boldsymbol{r}'$. So for large r we have

$$\begin{aligned}
\psi_t^{(+)}(\boldsymbol{r}) \sim \frac{1}{(2\pi)^{\frac{3}{2}}} \Bigg(&\exp(\mathrm{i}\,\boldsymbol{k}_i \cdot \boldsymbol{r}) - \sum_{ml} C_{ml} \pi \exp(\mathrm{i}\,kr)/r \\
&\times \int \mathrm{d}^3 r' \, \exp(-\mathrm{i}\,kr' \cos\theta) \exp(\mathrm{i}\,\mu_l kr' \cos\theta') \exp(-\lambda_m r')/r' \Bigg).
\end{aligned}$$

Expansion of the exponential terms in the integral and subsequent integration leads to the asymptotic form

$$\psi_t^{(+)}(\boldsymbol{r}) \sim \frac{1}{(2\pi)^{\frac{3}{2}}} \left(\exp(\mathrm{i}\,\boldsymbol{k}_i \cdot \boldsymbol{r}) + \frac{\exp(\mathrm{i}\,kr)}{r} \sum_n P_n(\cos\theta)\, \alpha_n \right), \tag{7}$$

where the α_n are functions of the parameters C_{ml}, λ_m and μ_l and may be considered arbitrary. Thus, the assumed form of the trial function has the nice property that asymptotically it also has the correct form. If one remembers the power of the least

squares principle and looks to the quality of the assumed trial form of the scattering state, it may be said that the present computational approach will give accurate converged results without meeting any major numerical instabilities. The method also is not very complicated and computations with a large number of terms in the trial function may readily be performed. Preliminary results of such a computation are reported in Section 3.

(b) Elastic Scattering of Electrons by Hydrogen Atoms

To illustrate how the computational scheme considered in Section 2*a* may be extended to other scattering problems of practical interest we consider here the computation of the direct scattering amplitude for elastic scattering of electrons by hydrogen atoms. The total Hamiltonian H in this case is decomposed as

$$H = H_0 + V = \{(-\nabla_1^2/2 - 1/r_1) - \nabla_2^2/2\} + (1/r_{12} - 1/r_2).$$

The direct scattering amplitude is expanded as

$$|\psi_i^{(+)}\rangle = |1s\, \boldsymbol{k}_i\rangle + \sum_n \int d^3q \, \frac{a_n(\boldsymbol{q})}{E - E_n(q) + i\epsilon} |n\boldsymbol{q}\rangle. \tag{8}$$

A convenient basis set for expansion of $a_n(\boldsymbol{q})$ may be $\{\langle n\boldsymbol{q}|\, V\lambda_m |1s\, \mu_l\, \boldsymbol{k}_i\rangle\}$, where $\langle n\boldsymbol{q}|\, V\lambda_m |1s\, \mu_l\, \boldsymbol{k}_i\rangle$ contain two real parameters λ_m and μ_l and in explicit terms

$$\langle n\boldsymbol{q}|\, V\lambda_m |1s\, \mu_l\, \boldsymbol{k}_i\rangle = \frac{1}{(2\pi)^3} \int \exp(-i\, \boldsymbol{q} \cdot \boldsymbol{r}_2)\, \phi_n(r_1)$$

$$\times \{\exp(-\lambda r_{12})/r_{12} - \exp(-\lambda r_2)/r_2\} \phi_{1s}(r_1) \exp(i\, \mu_l\, \boldsymbol{k}_i \cdot \boldsymbol{r}_2)\, d^3r_1\, d^3r_2, \tag{9}$$

where the $\phi_n(\boldsymbol{r})$ are hydrogenic states, and the λ_m may be chosen as 1, 2, 3, etc. (a.u.) and the μ_l may be chosen conveniently. The calculation then proceeds as before. Thus, one operates on equation (8) by $(E - H)$ giving

$$\begin{aligned}(E-H)|\psi_t^{(+)}\rangle &= -V|1s\, \boldsymbol{k}_i\rangle + \sum_n \int a_n(\boldsymbol{q})|n\boldsymbol{q}\rangle\, d^3q \\ &\quad - \sum_n \int \frac{a_n(\boldsymbol{q})}{E - E_n(q) + i\epsilon} V|n\boldsymbol{q}\rangle\, d^3q \\ &= -V|1s\, \boldsymbol{k}_i\rangle + \sum_{nml} C_{nml} \int |n\boldsymbol{q}\rangle\langle n\boldsymbol{q}|\, V\lambda_m |1s\, \mu_l\, \boldsymbol{k}_i\rangle\, d^3q \\ &\quad - \sum_{nml} C_{nml} \int \frac{V|n\boldsymbol{q}\rangle\langle n\boldsymbol{q}|\, V\lambda_m |1s\, \mu_l\, \boldsymbol{k}_i\rangle\, d^3q}{E - E_n(q) + i\epsilon}.\end{aligned} \tag{10}$$

The states $|\boldsymbol{p}_1\, \boldsymbol{p}_2\rangle$ form a complete set. We take the scalar product of equation (10) with $|\boldsymbol{p}_1\, \boldsymbol{p}_2\rangle$ and set the result equal to zero for determining the unknown variational parameters C_{nml}. So we have equations of the form

$$\sum_{nml} C_{nml}\, F_{nml}(\boldsymbol{p}_1, \boldsymbol{p}_2) - Y(\boldsymbol{p}_1, \boldsymbol{p}_2) = 0 \tag{11}$$

for parameters C_{nml}. Since integrations over a six-dimensional space will be very difficult and time consuming we propose choosing a large number of suitable points $(\boldsymbol{p}_{1i}, \boldsymbol{p}_{2j})$ in equation (11) and solving the resulting equations

$$\sum_{nml} C_{nml} F_{nml}(\boldsymbol{p}_{1i}, \boldsymbol{p}_{2j}) - Y(\boldsymbol{p}_{1i}, \boldsymbol{p}_{2j}) = 0, \tag{12}$$

for different points $(\boldsymbol{p}_{1i}, \boldsymbol{p}_{2j})$ by least squares principles. Thus we minimise

$$\sum_{ij} \left| \sum_{nml} C_{nml} F_{nml}(\boldsymbol{p}_{1i}, \boldsymbol{p}_{2j}) - Y(\boldsymbol{p}_{1i}, \boldsymbol{p}_{2j}) \right|^2 . \tag{13}$$

The minimising equations become

$$\sum_{nml} \left\{ \sum_{ij} F^*_{n'm'l'}(\boldsymbol{p}_{1i}, \boldsymbol{p}_{2j}) F_{nml}(\boldsymbol{p}_{1i}, \boldsymbol{p}_{2j}) \right\} C_{nml} = \sum_{ij} F^*_{n'l'm'}(\boldsymbol{p}_{1i}, \boldsymbol{p}_{2j}) Y(\boldsymbol{p}_{1i}, \boldsymbol{p}_{2j}), \tag{14}$$

for different $(n'm'l')$. The solution of these equations gives the estimated values C^*_{nml} of C_{nml}. Finally the T-matrix element is given by

$$T = \langle 1\mathrm{s}\, \boldsymbol{k}_\mathrm{f} | V | 1\mathrm{s}\, \boldsymbol{k}_\mathrm{i} \rangle + \sum_{nml} C^*_{nml} \int \mathrm{d}^3 q \, \langle 1\mathrm{s}\, \boldsymbol{k}_\mathrm{f} | V | n\boldsymbol{q} \rangle \times \langle n\boldsymbol{q} | V \lambda_m | 1\mathrm{s}\, \mu_l\, \boldsymbol{k}_\mathrm{i} \rangle . \tag{15}$$

An analysis similar to that described in Section 2*a* shows that the assumed trial wave function also has the correct asymptotic form.

Table 1. Comparison of the differential cross section in the present calculation for ten basis terms with those of other calculations

k_i	θ	First Born	Second Born	Das (1978)	Present work	Exact (Holt and Santoso 1973)
0·663	0	5·59	13·22	4·73	4·18	4·09
	$\frac{1}{2}\pi$	1·58	6·04	2·00	2·28	2·28
	π	0·74	3·92	1·41	2·28	2·29
1·816	0	5·59	7·08	4·96	5·41	5·33
	$\frac{1}{2}\pi$	0·097	0·293	0·126	0·123	0·127
	π	0·028	0·118	0·051	0·044	0·048
3·000	0	5·59	6·16	5·28	5·49	5·50
	$\frac{1}{2}\pi$	0·016	0·038	0·022	0·0189	0·0184
	π	0·004	0·013	0·007	0·0058	0·0052

3. An Application of the Computational Method

To study how the present least squares computational method works we undertook a computation of the scattering amplitude and the differential cross section for the Yukawa potential $V(r) = -1{\cdot}1825 \exp(-r)/r$. For this case exact results are also known (Holt and Santoso 1973) for certain values of the momentum and the scattering angle. We made a few different choices for the values of the parameters λ_m and μ_l. In one of these choices we have $\lambda_m = m$ and $\mu_l = l$ where m and l take the values 1, 2, 3, ... etc.