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

\[ |\psi_i^{(+)}\rangle = |k_i\rangle + \int d^3p \frac{a(q)}{E - E(q) + i\epsilon} |q\rangle, \quad (1) \]
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 $\theta$ 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 $\theta$ are unsuitable. We propose instead to use $1/\{(q - \mu_I k)^2 + \lambda_m^2\}$, with a discrete set of values for the parameters $\lambda_m$ and $\mu_I$, as basis functions in the momentum space. These are nothing but the Fourier transform of $\exp(-\lambda_m r)\exp(i\mu_I k \cdot r)/4\pi r$. It may be seen that a combination of these functions for different values of $\lambda_m$ and $\mu_I$ is sufficient to represent a function of the form $\Sigma_n R^{(\ast)}_n(r) P_n(\cos \theta)$ in which $R^{(\ast)}_n(r) \sim r^n$ near the origin. Now a choice of the parameters $\lambda_m$ 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 $\lambda_m$. A good choice for the $\mu_I$ 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

$$|\psi^{(+)}\rangle = |k_i\rangle + \sum_{ml} C_{ml} \int d^3 q \frac{|q\rangle}{[E - E(q) + i\epsilon] \{ (q - \mu_I k)^2 + \lambda_m^2 \}}, \quad (2)$$

where $C_{ml}$ are complex variational parameters.

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

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

$$- \sum_{ml} C_{ml} \int d^3 q \frac{V|q\rangle}{[E - E(q) + i\epsilon]\{ (q - \mu_I k)^2 + \lambda_m^2 \}}. \quad (3)$$

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:

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

$$- \sum_{ml} C_{ml} \int d^3 q \frac{\langle p | V | q \rangle}{[E - E(q) + i\epsilon]\{ (q - \mu_I k)^2 + \lambda_m^2 \}} = 0. \quad (4)$$

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

$$\int | \sum_{ml} C_{ml} F_{ml}(p) - Y(p) |^2 d\Omega_p. \quad (5)$$

The corresponding minimising equations are

$$\sum_{ml} \int d\Omega_p F_{ml}^*(p) F_{ml}(p) C_{ml} - \int d\Omega_p F_{ml}^*(p) Y(p) = 0,$$
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

\[
T = \langle k_f | V | \psi^{(+)}_t \rangle,
\]

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

\[
T = \langle k_f | V | k_i \rangle + \sum_{ml} C^*_{ml} \int d^3 q \frac{\langle k_f | V | q \rangle}{\left| \frac{E - E(q) + i\epsilon}{ \left( q - \mu_i k_i \right)^2 + \lambda_m^2 \right|}.
\]

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

\[
\psi^{(+)}_t(r) = \langle r | \psi^{(+)}_t \rangle
\]

\[
= \langle r | k_i \rangle + \sum_{ml} C_{ml} \int d^3 q \frac{\langle r | q \rangle}{\left| \frac{E - E(q) + i\epsilon}{ \left( q - \mu_i k_i \right)^2 + \lambda_m^2 \right|}
\]

\[
= \frac{\exp(\mu_i r)}{(2\pi)^{\frac{3}{2}}} + \sum_{ml} C_{ml} \int d^3 q \exp(\mu_i q \cdot r) \exp\left\{ -i(q - \mu_i k_i) \cdot r' \right\}
\]

\[
\times \exp\left( -\lambda_m r' \right)/(2\pi)^{\frac{3}{2}} \frac{1}{4\pi} \frac{\exp(-\lambda_m r')}{\left( q^2 - k^2 - i\epsilon \right)}
\]

\[
= \exp(\mu_i r)/(2\pi)^{\frac{3}{2}} - \sum_{ml} C_{ml} \int d^3 q d^3 r' \exp(\mu_i q \cdot R)
\]

\[
\times \exp(\mu_i k_i \cdot r') \exp\left( -\lambda_m r' \right)/(2\pi)^{\frac{3}{2}} \left( q^2 - k^2 - i\epsilon \right) r'.
\]

The \(q\) integration gives a factor \(2\pi^2 \exp(\mu_i R) R\), where \(R = | r - r' |\). Thus for \(r \to \infty\) we have \(R \approx r - r' \cos \theta\), where \(\theta\) is the angle between \(r\) and \(r'\). So for large \(r\) we have

\[
\psi^{(+)}_t(r) \sim \frac{1}{(2\pi)^{\frac{3}{2}}} \left( \exp(\mu_i r) - \sum_{ml} C_{ml} \pi \exp(\mu_i k_f r)/r \right.
\]

\[
\times \int d^3 r' \exp(-i k_f r' \cos \theta) \exp(\mu_i k_f r' \cos \theta') \exp(-\lambda_m r')/r'.
\]

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

\[
\psi^{(+)}_t(r) \sim \frac{1}{(2\pi)^{\frac{3}{2}}} \left( \exp(\mu_i r) + \frac{\exp(\mu_i k_f r)}{r} \sum_n P_n(\cos \theta) \alpha_n \right),
\]

where the \(\alpha_n\) are functions of the parameters \(C_{ml}, \lambda_m\) and \(\mu_i\) 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 2a 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

$$|\psi_1^{(+)}\rangle = |1s k_1\rangle + \sum_n \int d^3q \frac{a_n(q)}{E - E_n(q) + i\epsilon} |nq\rangle.$$

A convenient basis set for expansion of $a_n(q)$ may be $\langle nq | V\lambda_m | 1s \mu_i k_i \rangle$, where $\langle nq | V\lambda_m | 1s \mu_i k_i \rangle$ contain two real parameters $\lambda_m$ and $\mu_i$ and in explicit terms

$$\langle nq | V\lambda_m | 1s \mu_i k_i \rangle = \frac{1}{(2\pi)^3} \int \exp(-i\cdot q \cdot r_2) \phi_n(r_1) \times \{\exp(-\lambda r_{12})/r_{12} - \exp(-\lambda r_2)/r_2\} \phi_{1s}(r_1) \exp(i\mu_i k_i \cdot r_2) d^3r_1 d^3r_2,$$

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

$$(E - H)|\psi_1^{(+)}\rangle = -V|1s k_1\rangle + \sum_n \int a_n(q) |nq\rangle d^3q$$

$$- \sum_n \int \frac{a_n(q)}{E - E_n(q) + i\epsilon} V |nq\rangle d^3q$$

$$= -V|1s k_1\rangle + \sum_n C_{nml} \int |nq\rangle\langle nq | V\lambda_m | 1s \mu_i k_i \rangle d^3q$$

$$- \sum_n C_{nml} \int \frac{V |nq\rangle\langle nq | V\lambda_m | 1s \mu_i k_i \rangle d^3q}{E - E_n(q) + i\epsilon}.$$

The states $|p_1 p_2\rangle$ form a complete set. We take the scalar product of equation (10) with $|p_1 p_2\rangle$ and set the result equal to zero for determining the unknown variational parameters $C_{nml}$. So we have equations of the form

$$\sum_n C_{nml} F_{nml}(p_1, p_2) - Y(p_1, p_2) = 0$$
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
($p_{1i}, p_{2j}$) in equation (11) and solving the resulting equations

$$\sum_{nml} C_{nml} F_{nm}(p_{1i}, p_{2j}) - Y(p_{1i}, p_{2j}) = 0,$$

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

$$\sum_{ij} \sum_{nml} C_{nml} F_{nm}(p_{1i}, p_{2j}) - Y(p_{1i}, p_{2j})^{2}.$$  

The minimising equations become

$$\sum_{nml} \left\{ \sum_{ij} F^*_{nm} F_{n'm'}(p_{1i}, p_{2j}) F_{nm}(p_{1i}, p_{2j}) \right\} C_{nml} = \sum_{ij} F^*_{n'm'} Y(p_{1i}, p_{2j}),$$

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

$$T = \langle ls \ k_l | V | ls \ k_i \rangle + \sum_{nml} C^*_{nml} \int d^3 q \langle ls \ k_l | V | nq \rangle \times \langle nq | V \lambda_m | ls \ \mu_l \ k_i \rangle.$$  

An analysis similar to that described in Section 2a 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

<table>
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<th>$k_i$</th>
<th>$\theta$</th>
<th>First Born</th>
<th>Second Born</th>
<th>Das (1978)</th>
<th>Present work</th>
<th>Exact (Holt and Santos 1973)</th>
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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 $V(r) = -1.1825 \exp(-r)/r$. For this case exact results are
also known (Holt and Santos 1973) for certain values of the momentum and the
scattering angle. We made a few different choices for the values of the parameters
$\lambda_m$ and $\mu_l$. 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.