APPROXIMATE ANALYTIC WAVE FUNCTION METHOD IN ELECTRON ATOM SCATTERING CALCULATIONS

Budi Santoso*

ABSTRACT

APPROXIMATE ANALYTIC WAVE FUNCTION METHOD IN ELECTRON ATOM SCATTERING CALCULATIONS. Approximate analytic wave function method in the calculation of electron atom scattering cross sections have been developed. This method assumes that the dominant scattering amplitude is contributed by the static potential of the scattering process. The static potential is modeled such that the second Born off shell analytic form is available, i.e. in the form of screened Coulomb potentials. The potential strength parameters are determined from the variational Hartree-Fock method (Salvatz et al 1987). Approximate analytic wave function describing the scattering process in the static model can be obtained employing the Fredholm integral equation method developed by Holt and Santoso (1972). Using this wave function, any scattering process that is considered to be perturbing terms, can be calculated straightforward. This approximate wave function improves the Born approximation in that more wave numbers as a result of wave function spreading have been taken into account.

INTRODUCTION

Scattering processes have been a subject of interest even before the birth of quantum theory, since much information about the structure of matter can be derived from this study. With the development of quantum theory, more powerful tools for predicting interaction model in subatomic level can be explored. Within the framework of nonrelativistic quantum mechanics, a number of relatively simple potential models have been developed, i.e. square well, gaussian, screened coulomb and exponential potentials. Even with these simple models, exact calculations cannot be made readily available. Further approach need to be developed. Elaboration using direct numerical integration in the partial wave analysis approach has been used as a reference to other approaches. The partial wave approach has the advantage of more reliable in accuracy but with the drawback of acquiring numerous partial wave contributions have to be included in the calculations. A widely simple approach is the use of the Born approximation, with the main drawback that the results have uncertain accuracy. Improvement of the born approximation has been developed by Holt and Santoso (1974) by substituting the numerical values of the few lowest partial wave contributions. The convergence is fast, demonstrating that the accuracy obtained by partial wave method can be achieved by calculating only few lowest order only. Another approach that is complementary to the differential method is the integral method. In this approach the wave function is expanded in the form of fourier integral

* Nuclear Technology Assessment Centre, National Atomic Energy Agency (Batan)
termed as the Fredholm integral method, developed by Holt and Santoso (1973). This method has the advantage of presenting the wave function solution in an approximate analytic form, but with the drawback of dealing with relatively large dimension of simultaneous equation. Besides this, the off shell Born matrix elements need to be given analytically, otherwise the computation becomes too tedious. Moreover the methods given by Holt and Santoso above were limited only to central models that do not represent real system.

In the actual problem, the static potential approach is insufficient, because various atomic processes such as excitations, rearrangements, ionizations, stripping and others cannot be described using the simple models. One has to start by writing hamiltonian derived from the kinetic and coulomb potential energies. Further approximation is possible when one deals with simple system such as hydrogen or helium target atoms. Higher atomic numbers with more electrons involved can be dealt with statistical model. Recent interest in electron scattering problem have been given by Sienkiewicz et al. (1989), Macek et al (1994) and Fainstein (1996).

In the case of elastic scattering where a static central potential model can be employed, a systematic model derived from Hartree-Fock variational technique has been given by Salvat et al (1987). Combination of screened coulomb types with parameters have been given for all target atoms with atomic number 1 (hydrogen) to 92(uranium). This type of potential can be adopted in this method.

THEORETICAL FORMULATION

Let a beam of electrons scattered by a neutral target atom with the atomic number $Z$. The hamiltonian can be written as

$$\{-\frac{\hbar^2}{2m} \nabla^2 + H_a + V_{int}\} \Psi(\vec{r}, \vec{R}) = E\Psi(\vec{r}, \vec{R})$$

where $\vec{r}$ is the position of the electron projectile from the target nucleus (considered as the centre of mass of the system), $\vec{R} = \vec{r}_1, \vec{r}_2, \ldots, \vec{r}_Z$ describing the total coordinates of the $Z$ electron targets, $H_a$ is the hamiltonian of the target atom given by

$$H_a = \sum_{i=1}^{Z} \left\{ \left(-\frac{\hbar^2}{2m} \nabla_i^2 - \frac{Ze^2}{r_i} \right) + \frac{1}{2} \sum_{j=1}^{Z} \frac{e^2}{|\vec{r}_i - \vec{r}_j|} \right\}$$

satisfying $H_a \phi_a(\vec{R}) = \varepsilon_a \phi_a(\vec{R})$
and \( V_{\text{int}}(\vec{R}) \) is the potential interaction of electron projectile and the target atom given by

\[
V_{\text{int}}(\vec{R}) = -\frac{Ze^2}{r} + \sum_{i=1}^{Z} \frac{e^2}{|\vec{r} - \vec{r}_i|}
\]  
(4)

In principle the target wave functions and their eigen energies are known. A well known method of obtaining these are the Hartree-Fock variational techniques. It is therefore convenient to expand \( \Psi \) in term of \( \varphi_n \) given by

\[
\Psi(\vec{R}) = \sum_n F_n(\vec{r})\varphi_n(\vec{R})
\]  
(5)

so that after some rearrangement, equation (1) can be written as

\[
\{\nabla^2 + k_n^2\}F_n(\vec{r}) = \sum_m U_{nm}(r)F_m(\vec{r})
\]  
(6)

where \( k_n^2 = \frac{2m}{\hbar^2}(E - \epsilon_n) \) and \( U_{nm}(r) = \frac{2m}{\hbar^2}\int \varphi_m^*(\vec{R})V_{\text{int}}(\vec{r}, \vec{R})\varphi_n(\vec{R})d\vec{R} \)

In static approximation \( n=0 \) and \( U_{00} = 0 \) except for \( U_{00} \neq 0 \). This will simplify equation (6),

\[
\{\nabla^2 + k_0^2\}\psi(\vec{r}) = U(r)\psi(\vec{r})
\]  
(7)

where we have written \( \Psi = F_0 \) and \( U = U_{00} \). In general, one could try to approximate \( \sum_m U_{nm}(r)F_m(\vec{r}) = \tilde{U}(r)F_0(\vec{r}) \), where \( \tilde{U} \) is a complex potential.

Solution of equation (7) in an integral form is given by

\[
\psi(\vec{r}) = \exp(-ik_0\vec{r}) + \int G(\vec{r}, \vec{r}')U(r')\psi(\vec{r}')d\vec{r}'
\]  
(8)

For brevity it is written in the Dirac notation \( |\psi\rangle = |\vec{k}_0\rangle + GU|\psi\rangle \)

where the green function \( G(\vec{r}, \vec{r}') \) is given by

\[
G(\vec{r}, \vec{r}') = \frac{1}{(2\pi)^3} \int \frac{d\vec{p}}{p^2 - k_0^2 + i\epsilon_{p=0}} = -\frac{1}{4\pi} \frac{\exp(ik_0|\vec{r} - \vec{r}'|)}{|\vec{r} - \vec{r}'|}
\]  
(9)
Expanding $\psi(\vec{r})$ as

$$\psi(\vec{r}) = \int c(\vec{p}) \exp(\vec{i} \vec{p} \cdot \vec{r}) d\vec{p}$$  \hspace{1cm} (10)$$

and substitute this to equation (8), multiplying across with $\langle \vec{q} | U \rangle$ one obtains

$$\int c(\vec{p}) \langle \vec{q} | U - UGU | \vec{p} \rangle d\vec{p} = \langle \vec{q} | U | \vec{k}_0 \rangle$$  \hspace{1cm} (11)$$

For potentials of the form (Salvat et al 1987)

$$U(r) = \frac{Z}{r} \sum_{i=1}^{3} A_i \exp(-\alpha_i r)$$  \hspace{1cm} (12)$$

where $A_i$ and $\alpha_i$ are parameters given by Salvat et al (1987), the elements $\langle \vec{q} | U | \vec{p} \rangle$ and $\langle \vec{q} | UGU | \vec{p} \rangle$ can be evaluated analytically, i.e.

$$\langle \vec{q} | U | \vec{p} \rangle = Z \sum_{i=1}^{3} \frac{A_i}{(\vec{p} - \vec{q})^2 + \alpha_i^2}$$  \hspace{1cm} (13)$$

$$\langle \vec{q} | UGU | \vec{p} \rangle = Z^2 \sum_{i=1}^{3} \sum_{j=1}^{3} \frac{A_i A_j}{4\gamma^2 - C} \ln \left[ \frac{\gamma + \sqrt{\gamma^2 - C}}{\gamma - \sqrt{\gamma^2 - C}} \right]$$  \hspace{1cm} (14)$$

where

$$\gamma = \Lambda ((\vec{p} - \vec{q})^2 + \alpha_i \alpha_j + q^2 + \alpha_j^2) + \alpha_i (\Lambda^2 + p^2 + \alpha_j^2)$$

$$C = [(\vec{p} - \vec{q})^2 + (\alpha_i + \alpha_j)^2, [q^2 + (\alpha_i + \Lambda)^2, [p^2 + (\alpha_j + \Lambda)^2]$$

$$\Lambda = -i \kappa_0$$  \hspace{1cm} (15)$$

The only unknown in equation (11) is $c(\vec{p})$, and the integration can be approximated by point quadratures noting that

$$\int d\vec{p} = \int_0^{\infty} p^2 dp \int_{-1}^{1} d\cos \theta \int_{0}^{2\pi} d\phi$$  \hspace{1cm} . Since the potential interactions are centrally symmetrical function, the scattering amplitude is not function of $\phi$. Direct numerical integration can therefore be done over $\phi$, so that point quadratures are applied only for the other two integrations to give a simultaneous linear equation.
\[ \sum_{i=1}^{N} \sum_{j=1}^{M} A_{kl}c_{ij} = b_{kl} \]  

(16)

where \( N \) and \( M \) are the number of quadratures in the \( p \) and \( \cos(\vartheta_{pk_i}) \) integrations respectively and

\[
A_{kl} = \int_0^{2\pi} d\varphi \langle p_k,x_l|U - UGU|p_j,x_j \rangle \\
b_{ij} = \langle p_k,x_l|U|k_0,1 \rangle
\]

(17)

Solution of \( c_{ij} \) gives the analytic approximate solution for \( F_0 \) and hence \( \Psi \) which is

\[
\Psi(\vec{r}, \vec{R}) = F_0(\vec{r})\varphi_0(\vec{R})
\]

(18)

Scattering amplitude of any transition from the ground state to an excited state \( \varphi_n(\vec{R}) \) can be computed from

\[
f_{0n}(\Theta) = -\frac{1}{4\pi} \sum_{i=1}^{N} \sum_{j=1}^{M} c_{ij} \langle k_{ni},x_s|U_{0n}|p_j,x_j \rangle
\]

(19)

the matrix elements are understood to be integrated over \( d\varphi_{pk_i} \). This formulation improves the Born approximation in that the Born takes only one \( c_{ij} = \delta_{n_k} \delta_{j1} \).

RESULTS AND DISCUSSIONS

The method has been applied to the calculations of electron scattering by noble gas atoms. The \( k \)-integration quadratures have been chosen as \( k_1 = k_0, k_2 = 2k_0, k_3 = 0.5k_0, k_4 = 1.5k_0, k_5 = 0.75k_0, k_6 = 3k_0, k_7 = 4k_0 \) and so on, while \( x \)-quadratures are \( x_1 = 1, x_2 = -1, x_3 = 0, x_4 = 0.75, x_5 = -0.75, x_6 = 0.5, x_7 = -0.5 \) and so on. Table 1 presents the values of \( c_{ij} \) for \( N = 3, M = 4 \), while table 2 presents the values of total elastic scattering cross sections of electron scattering at 100 eV. As can be seen from this table, the values of the Born approximations are far from the converged values obtained numerically integrating the radial parts in the phase shift scheme, and hence they may not be expected to give good results for calculating any excitation process. The analytic representation wave function
method developed in these calculations however still give a good order of magnitudes even if only few number of point quadratures are used. The draw back of the method developed in this calculation is that the dimension of the linear equation to be solved escalates as $N^2 M^2$. An other problem would be related to the numerical stability of the ill conditioned in solving the linear equation.

REFERENCES

Table 1. The values $c_{ij} (N=3, M=4)$ of 100 eV e-He scattering, giving total elastic cross section $Q = 1.66$ (a.u.) compared to $Q(\text{Born}) = 1.46$ and $Q(\text{numeric}) = 1.74$

\[
\begin{array}{cccc}
1 & 2 & 3 & 4 \\
-2.0843 + 0.09898 i & 0.12102-0.12345 i & -0.31561-0.66737 i & 1.0927 +0.75204 i \\
0.34425+0.13243 i & -0.00061-0.13517 i & -1.3154 -0.56315 i & -0.50843+0.23654 i \\
7.6927 +1.1638 i & -0.16684+0.05026 i & 3.4999 +0.71476 i & -11.064 -1.8834 i \\
\end{array}
\]

Table 2. Total elastic cross sections (a.u) of 100 eV electron scattering

<table>
<thead>
<tr>
<th>Methods</th>
<th>He</th>
<th>Ne</th>
<th>Ar</th>
<th>Kr</th>
<th>Xe</th>
</tr>
</thead>
<tbody>
<tr>
<td>Numeric</td>
<td>1.74</td>
<td>7.32</td>
<td>15.22</td>
<td>10.58</td>
<td>12.46</td>
</tr>
<tr>
<td>Anal. (present)</td>
<td>1.91</td>
<td>8.13</td>
<td>26.65</td>
<td>30.68</td>
<td>48.30</td>
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<td>(N=7, M=8)</td>
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<tr>
<td>Born-1</td>
<td>14.61</td>
<td>22.43</td>
<td>95.99</td>
<td>233.5</td>
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<tr>
<td>Third Order</td>
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<td>76.64</td>
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