

Recurrence Relation for Integrals with Bessel Functions in Particle Scattering

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Uma fórmula de recorrência é desenvolvida para integrais envolvendo funções esféricas de Bessel do tipo $\int x^m e^{-\alpha x} j_k(sx) dx$ que assim podem ser calculadas usando-se

$$I_{a,s}(k+1,m) = \left(\frac{2k+1}{s}\right) I_{a,s}(k,m-1) - I_{a,s}(k-1,m)$$

$$I_{a,s}(k+1,m) = \int x^m e^{-\alpha x} j_{k+1}(sx) dx$$

onde $j_{k+1}(sx)$ são as funções esféricas de Bessel de ordem $k+1$.

It is shown that integrals equations involving Bessel functions such us $\int x^m e^{-\alpha x} j_k(sx) dx$ can be calculated using the following recurrence relation

$$I_{a,s}(k+1,m) = \left(\frac{2k+1}{s}\right) I_{a,s}(k,m-1) - I_{a,s}(k-1,m)$$

$$I_{a,s}(k+1,m) = \int x^m e^{-\alpha x} j_{k+1}(sx) dx$$

where $j_{k+1}(sx)$ are spherical Bessel functions. Calculations of integrals of this kind are particularly important in problems involving electron-atom and electron-molecule collisions.

Key words: *inelastic scattering; Bessel function; electron scattering; particle scattering.*

Introduction

The calculations of differential cross sections for atomic electron scattering and X-ray scattering has been the subject of many works found in the literature¹⁻¹⁰.

In general the problem can be divided into separate considerations of elastic and inelastic scattering. For the elastic part of the scattering the failure⁸⁻¹¹ of the first Born approximation has already been shown, especially at lower energies and for atoms of large atomic number. In the latter case improvement can be made by using the partial wave method, for example. However, for the inelastic part of the scattered amplitude we may expect that the Born approximation should provide a more suitable description¹².

Besides improving the method of treating the scattering process an improvement can also be made by using better wave functions to describe the scatterer⁵⁻⁹. This is especially true for the inelastic part because in the Born approximation it contains a term which strongly depends on the second order

density matrix which is very sensitive to electron correlation^{6,9,12,13}. Thus, for a careful comparison of theory with experiment, correlated wave functions should be used to calculate the scattering factors.

One of the ways to take into account electron correlation in the wave function is by the method of Configuration Interaction (CI) which despite its massive computational scheme is feasible for several atoms and simple molecular systems. On the other hand, current developments of experimental techniques in electron scattering have made it possible to compare experiment with theoretical differential cross sections for different wave functions. It is thus of more interest to obtain more accurate calculations in order to determine: a) the accuracy of the scattering theory employed, b) agreement between various atomic fields and the experiment, and c) details of the atomic charge cloud such as the Fourier transform for the electron pair correlation function^{12,14,15}.

In the framework of the Born approximation, the total electron scattered intensity by atoms can be written as

$$I(s) = \left(\frac{4s\beta_0}{a_0^2 s^4} \right) \{ [Z - F_x(s)]^2 + [Z - F_x^2(s) + \sum_{i \neq j} \sum_{i=1}^{NN} \langle \psi | e^{isr_{ij}} | \psi \rangle] \}$$

with $\beta_0 = 1 - (v/c)^2$, $a_0 = 0.529 \text{ \AA}^{-1}$, $F_x(s)$ is known as the X-ray form factor and $\Psi(r_1, \dots, r_N)$ is the many electron wave function for the atom. The first term in square brackets represents the elastic part of the scattered intensity, and the second term in square brackets is referred to as the inelastic scattering factor. Normally the evaluation of $F_x(s)$ is straight forward. However the same is not true for the inelastic part where the average $\langle \psi | \exp(isr_{ij}) | \psi \rangle$ must be evaluated. In this case, for each value of the momentum transfer s , we need to compute quite a large number of integrals such as

$$\int x^m e^{-\alpha x} j_k(sx) dx \quad (1)$$

for different values of m and k . Although the general solution for this integral can be solved directly to obtain

$$\int e^{-\alpha x} J_\lambda(sx) x^{\mu-1} dx = \sum \frac{(-1)^m (\frac{s}{2})^{\lambda+2m}}{m! \Gamma(\lambda+\mu+1)} \frac{\Gamma(\mu+\lambda+2m)}{a^{\mu+\lambda+2m}}$$

where

$$j_n(Z) = (\pi/2Z)^{1/2} J_{n+1/2}(Z)$$

this infinite serie is obviously not adequate for computing. Also, integration of (1) does not offer an especial advantage considering that, for larger values of k , we have to perform a great number of time consuming numerical integrations. Therefore a better method for solving (1) certainly will facilitate theoretical calculations involving electron-atom, electron-molecule and any other particle scattering where integrals of this type must be solved.

Method*

It is well known that spherical Bessel functions $j_k(z)$ can be obtained from the recurrence scheme¹⁷

$$j_{k+1}(z) = \frac{2k+1}{z} j_k(z) - j_{k-1}(z) \quad (2)$$

however, if we use this recurrence relation in (1) then we obtain

$$\int x^m e^{-\alpha x} j_{k+1}(sx) dx = \frac{2k+1}{s} \int x^{m-1} e^{-\alpha x} j_k(sx) dx - \int x^m e^{-\alpha x} j_{k-1}(sx) dx \quad (3)$$

Thus, making $I_{a,s}(k+1, m) = \int x^m e^{-\alpha x} j_{k+1}(sx) dx$, then

$$I_{a,s}(k+1, m) = \frac{2k+1}{s} I_{a,s}(k, m-1) - I_{a,s}(k-1, m) \quad (4)$$

However, to make use of this recurrence relation it is necessary the values for $I_{a,s}(-1, m)$ and $I_{a,s}(0, m)$; these can be solved quite easily to obtain¹⁸

$$I_{a,s}(0, m) = \frac{\Gamma(m)}{s(s^2+a^2)^{m/2}} \sin \{ m \tan^{-1}(s/a) \}$$

$$I_{a,s}(-1, m) = -\frac{\Gamma(m)}{s(s^2+a^2)^{m/2}} \cos \{ m \tan^{-1}(s/a) \}$$

The recurrence relation given by (4) is easier and more practical to handle in a computer than those given previously¹⁹, including the exact infinite series solutions mentioned.

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