المجلة العراقية للبحوث الإنسانية والإجتماعية والعلمية
Iraqi Journal of Humanitarian, Social and Scientific Research
Print ISSN 2710-0952 Electronic ISSN 2790-1254

A Study of Approximation Methods for Collision processes between Charged Particles and Atoms, Ions, or Molecules

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Abstract:

Atomic and molecular physics and chemistry are fundamentally dependent on the investigation of charged particle collisions. These collisions are crucial not only for industrial processes such as plasma technology, fusion energy, and radiation therapy, but also for understanding other natural phenomena, including ionization in Earth's atmosphere. This work aims to survey and evaluate various approximation methods used to analyses and understand collisions, emphasizing their practical applications across multiple scientific fields. This research investigated the subsequent methodologies: The Born Approximation is a first-order perturbation technique frequently utilized in weak potential scattering scenarios to calculate transition probabilities. It achieves this by considering the interaction as a negligible perturbation. The close-coupling approximation addresses complex collision scenarios by solving a system of coupled Schrödinger equations, accounting for the intense interactions between proximate particles.

Keywords: Collision processes, atoms, molecules, Born approximation, close-coupling approximation, quantum scattering.

دراسة طرق التقريب لعمليات التصادم بين الجسيمات المشحونة والذرات أو الأيونات أو الجزيئات

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الملخص:

تعتمد الفيزياء والكيمياء الذرية والجزيئية بشكل أساسي على التحقيق في تصادمات الجسيمات المشحونة. هذه التصادمات مهمة ليس فقط للعمليات الصناعية مثل تكنولوجيا البلازما، وطاقة الاندماج، والعلاج الإشعاعي، ولكن أيضًا لفهم الظواهر الطبيعية الأخرى، بما في ذلك التأين في الغلاف الجوي للأرض. يهدف هذا العمل إلى مسح وتقييم طرق التقريب المختلفة المستخدمة لتحليل وفهم التصادمات، مع التركيز على تطبيقاتها العملية عبر مجالات علمية متعددة. بحث هذا البحث في المنهجيات التالية: تقريب بورن هو تقنية اضطراب من الدرجة الأولى تُستخدم كثيرًا في سيناريوهات التشتت المحتمل الضعيف لحساب احتمالات الانتقال. ويحقق ذلك من خلال النظر إلى التفاعل باعتباره اضطرابًا لا يُذكر. يعالج التقريب الوثيق سيناريوهات التصادم المعقدة من خلال حل نظام من معادلات شرودنجر المقترنة، مع مراعاة التفاعلات الشديدة بين الجسيمات القريبة.

Print ISSN 2710-0952 Electronic ISSN 2790-1254

الكلمات المفتاحية: عمليات التصادم، الذرات، الجزيئات، تقريب بورن، تقريب الاقتران الوثيق، التشتت الكمومي.

Introduction

The study of charged particle, atomic, molecular, and ion collisions is fundamental to the understanding of many technological and natural processes and phenomena. A number of approximation techniques have been refined throughout the years to study and comprehend these crashes [1] . In an effort to present a thorough evaluation of these methods, this study will include a reference list that goes all the way back to the earliest studies in the subject and will focus on the work of important scholars who created these techniques [2] . When studying particle collisions, one of the first approximation approaches employed was the Born Approximation. Max Born proposed this approach in 1926[3], for systems with weak interactions; it determines transition probabilities by considering the interaction as a little perturbation. Its effectiveness and simplicity have made it useful in atomic and particle physics. Important studies that have used this approach include Tsitsi and Griffiths's (1999) and Kulik and Jacobsen's (1993) research. [4, 5].

To account for strong interactions between closely spaced particles, the Close-Coupling Approximation solves a system of coupled equations. Studying low-energy particle collisions, when interactions are substantial and cannot be ignored, requires this approach. Leading scholars in this area are James and Bolton (1990) and Williamson and Gallagher (1965) [6].

The Born approximation, the close-coupling approximation, and other analogous methods are commonly utilised to address inelastic processes in collision events involving charged particles interacting with atoms or molecules over a wide energy range [7, 8] .

Our publications[9-11] . in this filed were used the Born and Born-Bethe and other approximation methods were used to calculate the interaction cross sections and other issues[12-14] .

In previous research, we concentrated on the interactions of electrons and positrons with atoms and molecules, specifically calculating the elastic impact cross sections, annihilation parameters, and ionisation cross sections [15-19] .

The paper further contrasts theoretical outcomes with actual data, illustrating the efficacy of these approximation methods in forecasting cross-sections for atomic and molecular targets in excited collision processes. The findings indicate that

Print ISSN 2710-0952 Electronic ISSN 2790-1254

these methods not only improve theoretical comprehension but also have practical applications in fields such as plasma physics, particle physics, nuclear processes, and medical physics. This study underscores the essential function of approximation approaches in enhancing our understanding of particle interactions and their wider scientific ramifications.

Theory

This discussion will concentrate on two methodologies and demonstrate their efficacy in computing the inelastic differential cross sections for interactions between charged particles and atomic or molecular targets.

1. Born approximation

In the Born approximation, the differential cross section for scattering can be expressed using the following equation:

$$\frac{d\sigma}{d\Omega} = \left(\frac{m}{2\pi\hbar^2}\right)^2 |f(q)|^2$$

Where :

- $\frac{d\sigma}{d\Omega}$ is the differential cross section
- m is the mass of the particle.
- $\hbar$ is the reduced plank's constant.
- $f(q)$ is the scattering amplitude
- q is the momentum transfer, given by q=k-k`, where k and k` are the initial and final wave vectors of the particle.

The Scattering amplitude *f(q)* is given by the Fourier transform of the potential V(r) :

$$f(q)=\int e^{-iq.r}V(r)d^3r$$

The formulation is applicable to weak potential scattering where the Born potential scattering where the Born approximation is valid.

2. Close-Coupling approximation

Quantum scattering theory describes the scattering process using the differential cross section in the close-coupling approximation. As part of this process, a system of coupled channels' Schrodinger equation must be solved [20].

The basic form is given by:

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2$$

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Where the $f(\theta)$ is the scattering amplitude, which can be expressed in terms of partial waves and involves the solutions of the coupled –channel equations.

In the close- coupling approach, the scattering amplitude is calculated from

$$f(\theta) = \sum_{i=0}^{\infty}(2i+1)e^{i\delta_i}sin\delta_i P_i(cos\theta)$$

Here, δ_i are the phase shifts obtained from solving the coupled equations , and $P_i(cos\theta)$ are the Legendre polynomials.

The close- coupling method involves solving a set of coupled equations for the radial part of the wave function, which takes into account all relevant interactions and couplings between different channels.

Results

Here, we break down how to put the Born approach to work. Theoretical data for the rotating excitation transition from (0-0), (0-3) and (0-4) were compared with our DCS results at 5 eV in figure (1). Regarding Machado et al [19]. Brescansin et.al[21] , Jain et.al[22]. and the experimental data of Muller et.al[23].

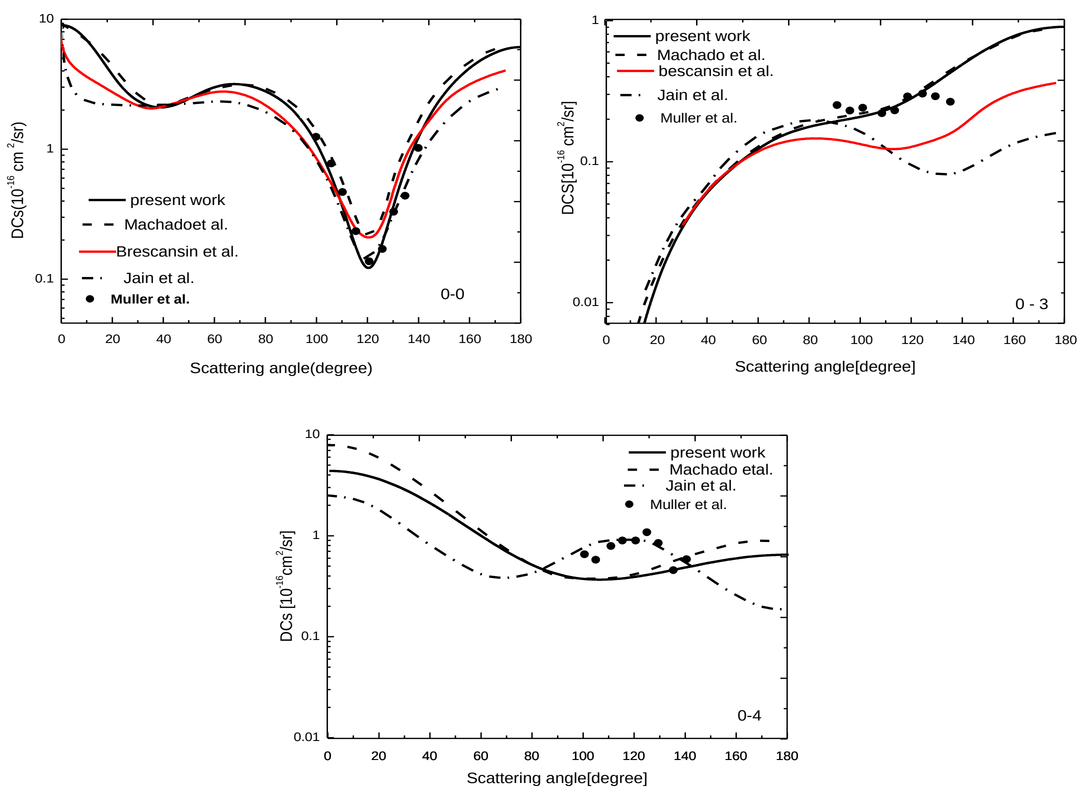

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Fig.1: Rotational excitation (J →J`) DCS for the e- CH_4 scattering at 5eV. The full curves are the present results. Other theoretical calculations are due to Machado [19], Brescansin [21], jain [22], And experimental Muller[23].

The application of close-coupling approach is explained in figure (2) [18], where it show how the DCS acts for both elastic and inelastic interaction for electrons collides with ionic Mg atom.

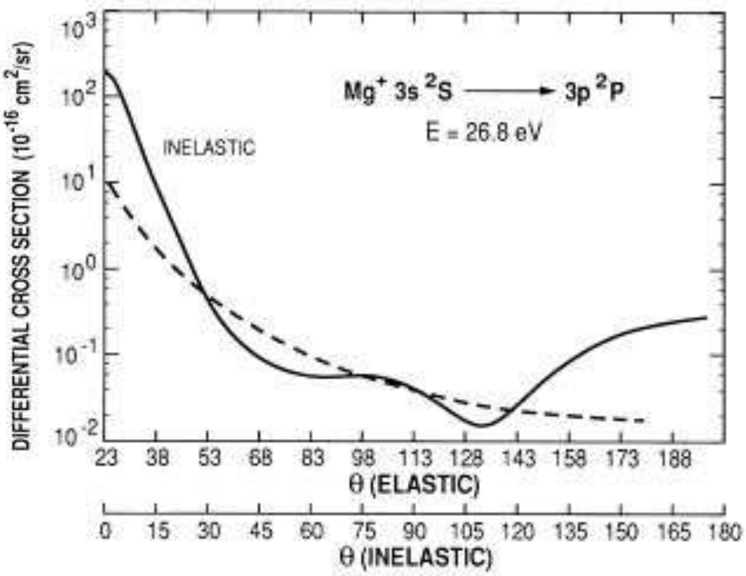

Fig. 2. Differential elastic and inelastic 3s →3p scattering cross sections for Mg+ at energy of 26.8 eV are from 5CC (HF).[24]

Conclusi

From the above, we conclude that the approximate methods we adopted showed good behavior for the cross sections of each of the targets with which the electrons collided, whether atomic or molecular. By comparing the results with the experimental and theoretical data, we have shown the effectiveness of using these approximate methods in the case of excited collisions.

In conclusion, the approximate methods discussed are indispensable tools for understanding and studying collisions between charged particles, atoms, and ions. By simplifying complex equations and enabling accurate analysis of particle behavior, these methods significantly enhance our theoretical understanding and practical applications in various scientific and technological fields. This comprehensive review underscores the importance of these methods in advancing our knowledge and highlights their practical applications across different domains such as plasma physics, particle physics, analytical chemistry, nuclear reactions, and medical research. We hope this study will serve as a valuable resource for

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researchers and contribute to further advancements in the field of collision analysis.

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