

Electron-molecule scattering with analytic static potential approach

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Abstract. A newly proposed analytic method to calculate static potential has been applied to study the elastic scattering of electron with CO_2 molecule. The molecule has been represented as a test case by using $STO-3G$ Gaussian wave functions initially. Results obtained for differential cross-section show good agreement when compared with experimental reported results.

1 Introduction

Optical potential model calculations have proved to be a very successful approach to study elastic electron-atom scattering. However, studying electron scattering from molecules using optical potential model calculations is complicated by the fact that molecules are a multi-centered target with the nuclei of the constituent atoms being a center of charge. Thus one of the most important parts of this scattering calculation is to obtain the static potential, which represents the interaction of the incident electron with the unperturbed charge distribution of the molecule. This job is very difficult and has been a challenge if multi-center wavefunctions are to be used for the molecular target.

Most of the calculations, therefore, used independent atom model where the electron-molecule scattering results are obtained by first considering the scattering of electron from the individual constituent atoms of the molecule and then getting the results for the molecule in approximate way whose reliability is questionable. In the present work, we adopt an approach where an analytic static potential is first generated from the multi-center molecular wavefunctions which can then be directly utilized in the optical potential method for studying the general case of electron scattering from molecules. Recently we have applied this analytical static potential approach to study electron scattering from water molecules represented by Gaussian wavefunctions [1]. Our method has given a very good description of electron-water molecule elastic scattering.

2 Results

In the present work we have extended our method in studying the elastic electron scattering from the linear molecule CO_2 using such an analytical static potential. We have obtained the spherically

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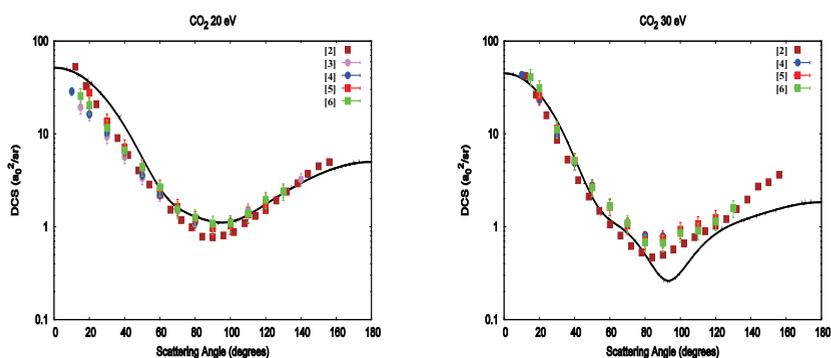


Figure 1. Differential cross-section of the elastic scattering of electron- CO_2 molecule at incident electron energy 20 and 30 eV.

symmetric part of the static interaction between an electron and CO_2 molecule represented by Gaussian wave functions. Since this molecule has no permanent dipole moment, we expect our method to produce accurate results for elastic scattering. As an illustration, we have presented our results for differential cross-section (DCS) of the elastic electron scattering of CO_2 molecule at electron impact energy 20 and 30 eV in the Figure 1. Our results are compared with existing experimental data [2–6] for this process to assess the accuracy of the method and we observed good agreement. Details of the method to obtain the static potential along with the description of full optical potential model can be followed from our earlier paper [1]. With the present work we show that it is possible to carry out the integrations analytically in order to find the spherically symmetric static potential due to the electronic charge distribution of an arbitrary molecule which is represented by Gaussian wavefunctions. Thus the accuracy of this potential is limited only by the accuracy of the molecular wavefunctions. Since our method is analytic, provided the molecule is represented by the well-known Gaussian wavefunctions, it can be applied to arbitrary molecular systems and requires much less in the way of computer resources than methods which depend on direct numerical integration of the wave function. There is no error in our method of evaluating of the static potential of the wave function and thus accurate Gaussian wavefunctions for a molecule will lead to correspondingly accurate potentials.

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