بسم الله الرحمن الرحيم

شبكة المعلومـــــات الجامعية

التوثيق الالكتروني والميكروفيلم

شبكة المعلومات الجامعية

جامعة عين شمس

التوثيق الالكتروني والميكروفيلم

﴿ قـــســـم ﴾

نقسم بالله العظيم أن المادة التي تم توثيقها وتسجيلها
علي هذه الأفلام قد اعدت دون آية تغيرات

يجب أن

تحفظ هذه الأفلام بعيداً عن الغبار

في درجة حرارة من 15 – 20 مئوية ورطوبة نسبية من 20-40 %

To be kept away from dust in dry cool place of
15 – 25c and relative humidity 20-40 %

بعض الوثائق الأصلية تالفة

بالرسالة صفحات

لم ترد بالأصـــل

EIGNVALUES PROBLEM IN VIEW OF THE THEORY OF COLLISION

THESIS

Submitted to the Faculty of Science

Zagazig University

BY

SAMIR MOHAMED HASSAN ALI

(M. Sc. Phys. 1987)

FOR

The Degree of Doctor of Philosophy In Physics

1994

CONTENTS

ACKNOWLEDGEMENT

The author wishes to thank ***Prof. Dr. A. H. Bassyouni,*** *Prof. of atomic physics, and Dean the Faculty of Science, Zagazig University, for supervision, kind help, and encouragement.*

I would like to express my thanks and deepest gratitude to ***Dr.H.A. Mourad,*** *Assistant Prof. of theoretical physics, Faculty of Science, Zagazig University, the author is sincerely grateful to him for suggesting the problem of research, close supervision, and careful discussion of the results during the progress of this study.*

The author wishes to express his appreciation to ***Prof. Dr. B. A. Tartoure,*** *Prof. of Nuclear Physics, and Vice-Dean for postgraduate studies, Faculty of Science, Zagazig University, for supervision, guidance, and kind help.*

Finally, my thanks to the staff members of the Department, for much assistance.

General Introduction

GENERAL INTRODUCTION

The motion of a single electron in the field of two complex atoms or ions constitutes a problem which is relevant for various topics in atomic and molecular physics. An important example is provided by ion-atom collisions with a relative nuclear velocity which is sufficiently small to allow the inner-shell or even outer-shell electrons to adjust their orbital motion to the momentary position of the two nuclei. In this way a transient quasimolecule is formed whose electronic energy levels vary with the internuclear separation during the collision.

In 1927, the molecular-orbital (MO) model was created by Hund[1] and Mulliken[2] to form a theoretical basis for molecular spectroscopy. In this model, the electrons were treated as independent particles. An important part of this model was electron promotion[1,2], in which the principal quantum number of certain MO's is higher in the united-atom (UA) limit than in the separated atom (SA).

In 1930, Beeck[3] observed sharp thresholds for the ionization of noble gases by impact with alkali-metal ions. Weizel and Beeck[4] interpreted these results in terms of electron promotion, with transitions at crossings of MO energy levels. They thought ionization occurred by Auger-electron emission when the electronic energy was raised into the ionization continuum, either directly during the collision or indirectly, after separation of the atoms has occurred.

In 1934, Coates[5] observed similar thersholds in inner-shell vacancy production and suggested a quasimolecular model to explain his resutls. Almost two decades after Weizel and Beeck's article, Moe and Petch[6] found Auger electrons in alkali-metal-ion-rare-gas collisions, and verified the indirect-ionization mechanism. A great deal of progress has been made in understanding the mechanism of heavy-particle collisions by the use of differential scattering measurements. Among the pioneers in this field were Fedorenko and Co-workers[7] and Everhart's group[8]. Inner-shell excitation in violent collisions was first studied in symmetric systems (Ar-Ar^+, Ne-Ne^+, Kr-Kr^+). Beeck[3,4] had found that the cross section for excitation was largest when both collision partners had nearly the same atomic number. Weizel and Beeck[4] interpreted this in terms of matching of atomic energy levels.

The concept of diabatic molecular states[9] has been used as a phenomenological models which can be compared with experimental data in a qualitative or semiquantitative way. These are made from antisymmetrized products of one-electron MO wave functions, can cross other states of the same symmetry, and can exist in the ionization continuum. Fano et al[10]. have extended this model to violent collisions, in which the atomic shells deeply penetrate each other[10,11]. This model assumes hydrogen-molecular-ion (H_2^+)-like MO's. During the collision, a quasimolecule is formed, in which the velocity of inner-shell electrons is much larger than the relative speed of the colliding heavy particles. The promoted electrons are trapped by crossings of promoted-inner-shell MO's with outer-shell MO's. The model gives a resonable interpretation of energy losses, inner-shell excitation, and characteristic internuclear distances for excitation and perturbation of elastic cross sections[12].

The question then arises of how to obtain reasonable diabatic correlation diagrams for arbitrary quasimolecular systems. The most promising approach to construct (quantitative) diabatic correlation diagrams consists in taking realistic adiabatic diagrams and making them diabatic. This is achieved by ignoring the gap between the energy curves at pseudocrossings and by drawing, in the crossing region, smooth connections which exhibit a real crossing.

For one electron in a field of two fixed nuclei, the rigorous rules of MO correlations have been obtained[13]. For the MO of multielectron quasimolecules, Barat and Lichten[14] suggested a simple rule for constructing diabatic correlations by considering the nodal structure of H_2^+-like electronic wave function. However, it was shown[15,16] that this rule leads to diagrams that do not contain many pseudocrossings of levels. On the basis of the results of numerical calculation of the one-electron energy terms of various quasimolecules, Eichler et al[17]. proposed another rule for MO correlation. Barat and Lichten[14] or Eichler et al[17]. rules is not sufficient for a unique determination of correlating MO. Therefore, Barat and Lichten[14], and Eichler et al[17]. introduced an additional rule according to which starting from the most strongly bound levels, each of the separated atom levels correlates to the lowest available (not yet occupied) level of the united atom.

Dowek et al.[18] have proposed an empirical method for determining the MO correlations of K-shell electrons of simple triatomic quasimolecules through the construction of "correlation cubes". Kereselidze and Kikiani[19] and Kereselidze[20] established rigorous rules for MO correlation of multielectron quasimolecules through the introduction of a screened two-centre one-electron effective potential and the representation of the molecular orbitals in the form of a linear combination of Coulomb MO.

Recently, Kereselidze[21] studied the motion of an electron in the field of three Coulomb centers where, the diabatic potential-energy surfaces of the system are found in the limit of united and separated atom.

In the present work, we analyzed a quasimolecule formed from one electron and three nuclei with charges $Z_1 = Z_2$ and $Z_3 = Z = 1, 2, 3,.....$ In Chap.1, we demonstrated that in spheroidal coordinate system when the distance between the foci is large, the Coulomb spheroidal quasiradial and quasiangular wave functions can be determined. In Chap.2, the diabatic potential energy surfaces of the quasimolecule are calculated when the distance L between the nucleus Z and the centre of the protons are large and small.

In Chap.3 we studied the transition probabilities as a function of the impact parameter and time in the two-state approximation at perpendicular and parallel orientation of H_2^+ molecule.

In Chap.4, we determin ed the exchange interaction potential of the H_2^+ molecule with bare nucleus, which are used to calculate the charge exchange cross section of the H_2^+ molecule on the nucleus of lithium atom.

Chapter I

CHAPTER I
COULOMB SPHEROIDAL WAVE FUNCTIONS

§ 1. Introduction :

The quantization problem of the hydrogen atom or hydrogen-like ion in prolate spheroidal coordinate system has been considered by many authors. Since the energy levels under quantization in any coordinate system are, obviously, the same, then the determination of the wave functions is the only requirement.

Various authors have determined the Coulomb Spheroidal wave functions, both directly, using an explicit form of the basis functions[22,23] and indirectly, using additional integrals of motions[24,25]. For a given n and m (where n is the principal quantum number; m is the magnetic quantum number) the problem reduces to the solution of a system of linear homogeneous algebraic equations of the order n-|m|. For small n-|m|, this system of equations can be solved analytically. However, for an arbitrary n-|m| and R, (R is the distance between the foci of spheroidal coordinate system) it is not possible to obtain a general solution.

The Coulomb spheroidal wave functions are defined, in general form, in two limiting cases; viz. large and small R. In the first case they are represented in the form of a linear combination of the Coulomb parabolic functions[22,25], while in the second case as a linear combination of the Coulomb spheroidal functions[25].

On solving many problems which arise in the physics of atomic collisions, e.g. for the evaluation of exchange interaction of the hydrogen atom with nuclei[26] and the form of nodal surface for two-centre system etc., it is necessary to know