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Dominant Correlation Effects in Two-Electron Atoms

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Abstract

Two-electron atoms have been investigated near threshold of double escape within the framework of hyperspherical coordinates. A particularly useful set of hyperspherical angles has been used. It is well known for many years that the hyperradial motion is nearly separable from the hyperspherical angular motion. Therefore, the Born-Oppenheimer separation method should be useful. However, the success of that method in molecular physics is based on the small mass ratio, electron mass to nuclear mass. In the atomic application such a small parameter does not exist. Nevertheless the method works surprisingly well in the lower part of the spectrum. For increasing excitation energy the method becomes shaky. Near ionization threshold, it breaks even down. The author will present elsewhere an improved Born-Oppenheimer method. First pilot developments and comparison with the experimental situation are presented already here. Inclusion of a momentum-momentum radial coupling delivers an improved basis. We show that our extended Born-Oppenheimer approach leads to a deformation of the whole potential energy surface during the collision. In consequence of this deformation we outline a quantum derivation of the Wannier threshold cross section law, and we show that (e, 2e) angular distribution data are strongly influenced by that surface deformation. Finally, we present a mechanism for electron pair formation and decay leading to a supercurrent independent of the temperature. Our framework can be extended to more than two electrons, say 3 or 4. We conclude that our improved Born-Oppenheimer method [1] is expected not only to deliver better numerical data, but it is expected to describe also the Wannier phenomenon. The idea of the new theory together with first qualitative results is presented in this paper.

Keywords

Born-Oppenheimer Approximation, Wannier Theory, Electronic Correlation, 3-Body Systems, Hyperspherical Coordinates

Correlation Effects In Atoms Molecules

J.P. Connerade, J.M. Esteva, R.C. Karnatak

Correlation Effects In Atoms Molecules:

Correlation Effects in Atoms and Molecules R. Lefebyre, C. Moser, 1969 Cumulative index to volumes I XIV Atomic. Molecular, and Optical Physics National Research Council, Division on Engineering and Physical Sciences, Commission on Physical Sciences, Mathematics, and Applications, Board on Physics and Astronomy, Physics Survey Committee, Panel on Atomic, Molecular, and Optical Physics, 1986-02-01 The goals of atomic molecular and optical physics AMO physics are to elucidate the fundamental laws of physics to understand the structure of matter and how matter evolves at the atomic and molecular levels to understand light in all its manifestations and to create new techniques and devices AMO physics provides theoretical and experimental methods and essential data to neighboring areas of science such as chemistry astrophysics condensed matter physics plasma physics surface science biology and medicine It contributes to the national security system and to the nation's programs in fusion directed energy and materials research Lasers and advanced technologies such as optical processing and laser isotope separation have been made possible by discoveries in AMO physics and the research underlies new industries such as fiber optics communications and laser assisted manufacturing These developments are expected to help the nation to maintain its industrial competitiveness and its military strength in the years to come This report describes the field characterizes recent advances and identifies current frontiers of research Collision Theory Richard Barry Bernstein, 2013-11-11 The broad field of molecular collisions is one of considerable current interest one in which there is a great deal of research activity both experimental and theoretical This is probably because elastic inelastic and reactive intermolecular collisions are of central importance in many of the fundamental processes of chemistry and physics One small area of this field namely atom molecule collisions is now beginning to be understood from first principles Although the more general subject of the collisions of polyatomic molecules is of great im portance and intrinsic interest it is still too complex from the viewpoint of theoretical understanding However for atoms and simple molecules the essential theory is well developed and computational methods are sufficiently advanced that calculations can now be favorably compared with experimental results This coming together of the subject and incidentally of physicists and chemists though still in an early stage signals that the time is ripe for an appraisal and review of the theoretical basis of atom molecule collisions It is especially important for the experimentalist in the field to have a working knowledge of the theory and computational methods required to describe the experimentally observable behavior of the system By now many of the alternative theoretical approaches and computational procedures have been tested and intercompared More or Iess optimal methods for dealing with each aspect are emerging In many cases working equations even schematic algorithms have been developed with assumptions and caveats delineated The Effects of Relativity in Atoms, Molecules, and the Solid State Stephen Wilson, I.P. Grant, B.L. Gyorffy, 2012-12-06 Recent years have seen a growing interest in the effects of relativity in atoms molecules and solids On the one hand this can be seen as result of the growing awareness of the importance of

relativity in describing the properties of heavy atoms and systems containing them This has been fueled by the inadequacy of physical models which either neglect relativity or which treat it as a small perturbation On the other hand it is dependent upon the technological developments which have resulted in computers powerful enough to make calculations on heavy atoms and on systems containing heavy atoms meaningful Vector processing and more recently parallel processing techniques are playing an increasingly vital role in rendering the algorithms which arise in relativistic studies tractable This has been exemplified in atomic structure theory where the dominant role of the central nuclear charge simplifies the problem enough to permit some prediction to be made with high precision especially for the highly ionized atoms of importance in plasma physics and in laser confinement studies Today's sophisticated physical models of the atom derived from quantum electrodynamics would be intractable without recourse to modern computational machinery Relativistic atomic structure calculations have a history dating from the early attempts of Swirles in the mid 1930 s but continue to provide one of the primary test beds of modern theoretical physics **Correlation Effects in Atoms and Molecules, Volume 14** W. Curt Lefebvre, 2009-09-08 The Advances in Chemical Physics series provides the chemical physics and physical chemistry fields with a forum for critical authoritative evaluations of advances in every area of the discipline Filled with cutting edge research reported in a cohesive manner not found elsewhere in the literature each volume of the Advances in Chemical Physics series serves as the perfect supplement to any advanced graduate class devoted to the study of chemical physics Polarizabilities of Atoms, Molecules, and Clusters Keith D. Bonin, Vitaly V. Kresin, 1997 This book is an in depth review of experiment and theory on electric dipole polarizabilities. It is broad in scope encompassing atomic molecular and cluster polarizabilities Both static and dynamic polarizabilities are treated in the absence of absorption and a full tensor picture of the polarizability is used Traditional experimental techniques for measuring electric polarizabilities are described in detail Recently developed experimental methods including light forces position sensitive time of flight deflection and atom interferometry are also extensively discussed Theoretical techniques for calculating polarizabilities are reviewed including a discussion on the use of Gaussian basis sets Many important comparisons between theory and experiment are summarized in an extensive set of tables of polarizabilities of important atoms molecules and clusters Applications of polarizabilities to many areas of chemistry and physics are described including optics chemical structure interactions of gases and particles with surfaces and the interaction of molecules with light The emphasis is on a lucid presentation of the ideas and results with up to date discussions on important applications such as optical tweezers and nanostructure fabrication This book provides an excellent overview of the importance of polarizabilities in understanding the physical electronic and optical properties of particles in a regime that goes from free atoms to condensed phase clusters **Correlation Effects in Atoms and Molecules** Roland Lefebvre, C. Moser, 1969 Cumulative index to volumes I XIV Relativistic Theory of Atoms and Molecules Pekka Pyykkö, 2012-12-06 Atoms, Molecules and Clusters in Electric Fields George Maroulis, 2006 With the

central importance of electric polarizability and hyperpolarizability for a wide spectrum of activities this book charts the trends in the accurate theoretical determination of these properties in specialized fields The contributions include reviews and original papers that extend from methodology to applications in specific areas of primary importance such as cluster science and organic synthesis of molecules with specific properties Relativistic and Electron Correlation Effects in Molecules and Solids G.L. Malli, 2013-11-21 The NATO Advanced Study Institute ASI on R lativistic and Electron Correlation Effects in Molecules and Solids co sponsored by Simon Fraser University SFU and the Natural Sciences and Engineering Research Council of Canada NSERC was held Aug 10 21 1992 at the University of British Columbia UBC Vancouver Canada A total of 90 lecturers and students with backgrounds in Chemistry Physics Mathematics and various interdisciplinary subjects attended the ASI In my proposal submitted to NATO for financial support for this ASI I pointed out that a NATO ASI on the effects of relativity in many electron systems was held ten years ago See G L Malli ed Relativistic Effects in Atoms Molecules and Solids Plenum Press Vol B87 New York 1983 Moreover at a NATO Advanced Research Workshop ARW on advanced methods for molecular electronic structure an assessment of state of the art of Electron Correlation was carried out see C E Dykstra ed Advanced Theories and Computational Approaches to the Electronic Structure of Molecules D Reidel Publishin Company Vol C133 Dordrecht The Netherlands 1984 However during the last five years it has become clear that the relativistic and electron correlation effects must be included in the theoretical treatment of many electron molecules and solids of heavy elements with Z 70 Molecules and clusters containing heavy elements are of crucial importance in a number of areas of Chemistry and Physics such as nuclear fuels catalysis surface science etc Advances in Atomic, Molecular, and Optical Physics ,1992-02-03 Advances in Atomic Molecular and Optical Physics **Methods in Computational Molecular Physics** Stephen Wilson, Geerd H.F. Diercksen, 2013-11-11 This volume records the lectures given at a NATO Advanced Study Institute on Methods in Computational Molecular Physics held in Bad Windsheim Germany from 22nd July until 2nd August 1991 This NATO Advanced Study Institute sought to bridge the quite considerable gap which exist between the presentation of molecular electronic structure theory found in contemporary monographs such as for example McWeeny s Methods 0 Molecular Quantum Mechanics Academic Press London 1989 or Wilson's Electron correlation in molecules Clarendon Press Oxford 1984 and the realization of the sophisticated computational algorithms required for their practical application It sought to underline the relation between the electronic structure problem and the study of nuclear motion Software for performing molecular electronic structure calculations is now being applied in an increasingly wide range of fields in both the academic and the commercial sectors Numerous applications are reported in areas as diverse as catalysis and interstellar chernistry drug design and environmental studies molecular biology and solid state physics The range of applications continues to increase as scientists recognize the importance of molecular structure studies to their research activities Recent years have seen a growing dependence of these applications on program packages which are often not in the public domain

and which may have a somewhat limited range of applicability dicta ted by the particular interests and prejudices of the Giant Resonances in Atoms, Molecules, and Solids J.P. Connerade, J.M. Esteva, R.C. Karnatak, 2013-12-20 Often a new area of science grows at the confines between recognised subject divisions drawing upon techniques and intellectual perspectives from a diversity of fields Such growth can remain unnoticed at first until a characteristic fami ly of effects described by appropriate key words has developed at which point a distinct subject is born Such is very much the case with atomic giant resonances For a start their name itself was borrowed from the field of nuclear collective resonances. The energy range in which they occur at the juncture of the extreme UV and the soft X rays remains to this day a meeting point of two different experimental techniques the grating and the crystal spectrometer The impetus of synchrotron spectroscopy also played a large part in developing novel methods described by many acronyms which are used to study giant resonances today Finally although we have described them as atomic to differentiate them from their counterparts in Nuclear Physics their occurrence on atomic sites does not inhibit their existence in molecules and solids In fact giant resonances provide a new unifying theme cutting accross some of the traditional scientific boundaries After much separate development the spectroscopies of the atom in various environments can meet afresh around this theme of common interest Centrifugal barrier effects and giant resonances proper emerged almost simultaneously in the late 1960 s from two widely separated areas of physics namely the study of free atoms and of condensed matter Frontiers in Atomic, Molecular and Optical Physics, Vol. 3, 2003 Atoms, Molecules and Photons Wolfgang Demtröder, 2019-02-09 This introduction to Atomic and Molecular Physics explains how our present model of atoms and molecules has been developed over the last two centuries both by many experimental discoveries and from the theoretical side by the introduction of quantum physics to the adequate description of micro particles It illustrates the wave model of particles by many examples and shows the limits of classical description The interaction of electromagnetic radiation with atoms and molecules and its potential for spectroscopy is outlined in more detail and in particular lasers as modern spectroscopic tools are discussed more thoroughly Many examples and problems with solutions are offered to encourage readers to actively engage in applying and adapting the fundamental physics presented in this textbook to specific situations Completely revised third edition with new sections covering all actual developments like photonics ultrashort lasers ultraprecise frequency combs free electron lasers cooling and trapping of atoms quantum optics and quantum information Advances in Atomic, Molecular, and Optical Physics Paul R. Berman, Ennio Arimondo, Chun C. Lin, 2011-10-03 Advances in Atomic Molecular and Optical Physics publishes reviews of recent developments in a field which is in a state of rapid growth as new experimental and theoretical techniques are used on many old and new problems Topics covered include related applied areas such as atmospheric science astrophysics surface physics and laser physics Articles are written by distinguished experts and contain both relevant review material and detailed descriptions of important recent developments International experts Comprehensive articles New developments Springer

Handbook of Atomic, Molecular, and Optical Physics Gordon W. F. Drake, 2023-02-09 Comprises a comprehensive reference source that unifies the entire fields of atomic molecular and optical AMO physics assembling the principal ideas techniques and results of the field 92 chapters written by about 120 authors present the principal ideas techniques and results of the field together with a guide to the primary research literature carefully edited to ensure a uniform coverage and style with extensive cross references Along with a summary of key ideas techniques and results many chapters offer diagrams of apparatus graphs and tables of data From atomic spectroscopy to applications in comets one finds contributions from over 100 authors all leaders in their respective disciplines Substantially updated and expanded since the original 1996 edition it now contains several entirely new chapters covering current areas of great research interest that barely existed in 1996 such as Bose Einstein condensation quantum information and cosmological variations of the fundamental constants A fully searchable CD ROM version of the contents accompanies the handbook **Current Developments in Atomic, Molecular,** and Chemical Physics with Applications Man Mohan, 2012-12-06 Proceedings of an International Conference on Current Developments in Atomic Molecular and Chemical Physics with Applications held March 20 22 2002 in Delhi India The 38 chapters cover a broad range of research activities categorized into four sub topics namely Processes in Laser Fields Chemical Physics Collision Processes Atomic Structure and Applications Lasers in Atomic, Molecular, and Nuclear Physics V. S. Letokhov, 1986 Current Topics in Atomic, Molecular and Optical Physics Indian Association for the Cultivation of Science, 2007 Focuses on research in crucial areas such as cold atoms and Bose Einstein condensates quantum information and quantum computation and techniques for investigating collisions and structure This work covers topics that includes the multireference coupled cluster method in quantum chemistry and the role of electronic correlation in nanosystems

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