Progress Report for the period Sept. 1, 1990 to Nov. 30, 1991
Physics of Correlated Systems

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H⁻ Doubly-Excited State Properties

Building on past successes in treating electron correlation in two-electron systems using eigenchannel R-matrix methods and multichannel quantum defect techniques (MQDT), the P.I. has recently collaborated with H. Sadeghpour and M. Cavagnero to extend these calculations to deal with resonant H⁻ photodetachment.¹ A new feature of these calculations is the use of the Gailitis-Damburg dipole representation in conjunction with generalized MQDT for dipole fields. The resulting calculations have reproduced H⁻ photodetachment spectra observed at LAMPF up to the $N = 4$ threshold, to within experimental errors. Moreover, a study of the dominant eigenstate of the time-delay matrix near each resonance confirms a qualitative selection rule suggested by the P.I. and Sadeghpour a year ago using hyperspherical coordinate methods. (Analogous selection rules had previously been proposed and developed by Herrick, Lin, Watanabe, Briggs, and others.) Thus, for example, this study of time-delay eigenstates has shown that the main $^1P^o$ "Wannier ridge resonance" lying below the $N = 4$ threshold, having no bending vibrational quanta ($v^A = 0^+$), decays 73% of the time into the $N = 3$ hydrogenic continuum with $v^A = 0^+$ and 18% of the time into the similar $N = 2$ continuum. The approximate selection rules which had been proposed on qualitative grounds from adiabatic hyperspherical studies, molecular-type models, and group-theoretical methods, are thus verified and given a quantitative range of validity.

Spectra of Heavy Open-Shell Atoms

A major effort in this contract is underway in an effort to develop improved theoretical methods capable of predicting the properties of complex open-shell atoms. Some progress in recent years has been achieved both by the P.I. and by M. Aymar in using eigenchannel R-matrix techniques in conjunction with a semiempirical model potential. This formulation is capable of efficiently calculating the short-range parameters which are subsequently used in a standard MQDT calculation to predict the photoabsorption or collision spectrum. To date, this method has primarily been tested in all of the alkaline earth atoms (including radium), where a range of experimental tests has shown the resulting MQDT parameters to be unexpectedly accurate and reliable.

In the short time F. Robicheaux has been a postdoctoral research associate on this project (since December 1990), he has independently written a new eigenchannel R-matrix computer program capable of handling many LS -coupled electrons in one or more open shells. While much of the technology for handling such many-electron matrix elements are familiar in the literature, adapting this

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technology into the eigenchannel approach nevertheless required a nontrivial effort. Test calculations in aluminum and boron photoionization indicate that the method works, and that it can deal efficiently with the strong hybridization of orbitals resulting from nonperturbative electron correlation effects. Studies of more complex atoms are in progress.

A fraction of Robicheaux's effort has been diverted profitably into a collaboration with Bo Gao, another JILA research associate, in developing a new formulation for multiphoton ionization calculations. The new formulation, while treating the atom-light interaction at the level of perturbation theory, can treat the strongly nonperturbative electron correlation physics at a level of accuracy comparable to that achieved in one-photon absorption spectra of the alkaline earth atoms. Specifically, Robicheaux and Gao² have extended eigenchannel R-matrix methods and MQDT so as to handle inhomogeneous wave equations of the type which routinely occur in the Dalgarno-Lewis approach to perturbation theory. Pilot calculations for multiphoton ionization of aluminum and for several of the alkaline earth atoms appear to be the most reliable to date. They are now beginning to show systematic trends of the autoionizing levels in their dual role as both intermediate states and as final states in multiphoton absorption processes.

Atomic Hydrogen in a Strong Magnetic Field

A student working on this project, Qiaoling Wang, has made substantial progress in understanding quantitatively the nature of the absorption spectrum at superstrong magnetic fields not realizable in the laboratory ($B \geq 10^3$ Tesla). Wang's converged calculations have been conducted using an eigenchannel R-matrix method set up inside a cylindrical box, with a standard MQDT channel expansion applied outside the box. One key element of these calculations has been the inclusion of not only cylindrical variational basis functions, but also several Sturmian functions having spherical symmetry which improve the flexibility of the trial wavefunctions near the nucleus. Extrapolations suggest that in their present form, such calculations are still not sufficiently efficient to allow treatment of laboratory-strength fields in the $6T$ range. In the meantime, more elegant frame transformation techniques have been developed independently by S. Watanabe and by P. O'Mahony, which are far more successful and efficient at these laboratory-strength magnetic fields, and they have confirmed the usefulness of an MQDT description of the spectrum.

In the past year, Q. Wang has made rapid progress, resulting in two publications with the P.I.^{3,4} The first of these formulates the general features to be expected whenever the thresholds in a multichannel Rydberg spectrum vary as functions of a tunable parameter such as the magnetic field strength. This paper has shown how many of the features seen by the Kleppner group must generally be present in such a parameter-dependent Rydberg spectrum. The second paper presents detailed R-matrix calculations of photoionization spectra for hydrogen, in the range of magnetic fields $10^3 T - 10^4 T$. These calculations show how the spectrum becomes increasingly complicated as the magnetic field is decreased, leading to the formation of quasi-Landau-type resonances which can be viewed as short-range perturbations (in their extent parallel to the field). A novel prediction of this work, which should be applicable even at laboratory-strength fields,

is that the branching ratio for photoionization into the different available Landau channels behaves completely differently for final states with $m = 0$ and $m = 1$. In particular, if a low-lying s -state of a one-electron atom is photoionized with circularly polarized light along the field, the highest accessible Landau channels tend to be excited, while light polarized linearly along the field tends to excite the lowest available Landau channels. A Ph.D. will be completed in August 1991 by Q. Wang based on this research.

Other Simple Atomic Systems

Other fundamental systems to be investigated under this project include triply-excited states of H^{-} and also the positronium molecule Ps_2 . In the first of these, a major question is still whether resonances exist above the threshold energy for escape of all electrons to infinity. This and related questions have been studied by a new graduate student R. Wood, who has spent several months but with no concrete results to report as yet.

References

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