THEORETICAL STUDIES OF HIGHLY IONIZED SPECIES

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Abstract

The relativistic random phase approximation has been used to study the helium, beryllium, magnesium and zinc isoelectronic sequences. Model potential methods have been employed to study multi-photon ionization of sodium from the ground and excited states. Forbidden decays in the Be and Mg isoelectronic sequences have been investigated. The $1s2p^2\ ^2P$ and $1s2p^2\ ^2D$ states of lithium-like ions have been studied. Calculations of radiative charge transfer have been carried out.

1. Introduction

We have been engaged in a wide range of activities in theoretical research in atomic and molecular physics that relate to the mission of the Basic Energy Sciences Division of the Office of Energy Research of the Department of Energy. We follow the form of our previous report and place our activities into several distinct categories, which we discuss in turn.

2. Applications of the relativistic Random Phase Approximation

The random phase approximation or equivalently time-dependent Hartree-Fock theory has been widely used in the study of allowed electric dipole transitions in atoms and molecules of low nuclear charge (cf. Amusia and Cherepkov 1975, Stewart 1975, Stewart, Watson and Dalgarno 1975, 1976, Yeager, Nascimento and McKoy 1975, Watson, Stewart and Dalgarno 1976) that can be described by the L-S coupling scheme. The approximation is remarkably accurate. For large nuclear charges relativistic effects are significant and in order to treat such systems we introduced a relativistic generalization (W. R. Johnson and A. Dalgarno 1975 unpublished) of the random phase approximation that permits the non-perturbative incorporation of relativistic effects and extends the theory to allowed and forbidden transitions of all multipolarities. The method automatically provides the correct angular momentum coupling scheme. We have now calculated the $E1(S^1, {}^3P_1 - 1^1S_0)$, $M1(2^3S_1 - 1^1S_0)$ and $M2(2^3P_2 - 1^1S_0)$ transition probabilities of the entire helium sequence (Johnson, Lin and Dalgarno 1976, Johnson and Lin 1976) and we have extended the method to the calculations of E1 transitions between excited states

(Lin, Johnson and Dalgarno 1977). For Fe and Ni we have calculated relativistic transition probabilities of all levels up to $n=5$ (Lin, Johnson and Dalgarno 1977).

We have now carried out complete studies of the beryllium isoelectronic sequence (Lin and Johnson 1977). By freezing the inner shells, we were able to treat expeditiously the valence transitions of the magnesium (Shorer, Lin and Johnson 1977) and zinc isoelectronic sequences (Shorer and Dalgarno 1977) and we have recently shown by perturbation methods that relaxation of the d-shell electrons in the zinc sequence has but a small effect on resonance transitions of the zinc 4s electrons (Shorer 1977). We have now developed a systematic treatment amenable to numerical solution that incorporates all the electrons on an equal basis.

We have carried out (Watson, Stewart and Dalgarno 1977) preliminary studies of the non-relativistic background photoionization continuum using the Stieltjes imaging method for the beryllium isoelectronic sequence. The method works well but our recent numerical development may mean that a direct numerical attack would be more attractive. Some results for neutral beryllium within the relativistic random-phase approximation have been published for the outer shell photoionization (Johnson and Lin 1977) but the inner shell resonance structures which appear so clearly in the non-relativistic close-coupling calculations by Bely-Dubau, Dubau and Petrini (1977) have yet to be studied.

3. Model Potential Methods

Model potential methods provide a simple way of accurately predicting those properties of atomic and molecular systems which depend mainly on the outer shell valence electrons. They are particularly useful in assessing the accuracy of other approximations which do not contain a comprehensive description of the valence shell electron interactions.

Model potential methods have been used to calculate the probabilities of the magnetic quadrupole transitions $^3P_2^0 - ^1S_0$ for the beryllium and magnesium isoelectronic sequences (Lin, Laughlin and Victor 1977). The results show that an often used "single configuration" approximation is of low accuracy.

The decay of the $^3P_0^0$ metastable state of beryllium-like ions has been investigated using lowest order perturbation theory expansion in Z^{-1} , where Z is the nuclear charge (Laughlin and Johnson 1978). The state decays very slowly because it is a two-photon process, where one of the photons is of the magnetic dipole type, and the other photon is of the spin-forbidden electric dipole type.

Accurate one- and two-photon ionization rates for the ground and excited states of sodium have been calculated (Laughlin 1978). The results are obtained using a combination of explicit summation over nearby intermediate states with the remainder of the sum being evaluated using an inhomogeneous

differential equation method. A large two-photon ionization rate is found for the 3p level of sodium irradiated by a laser tuned to the sodium D resonance line. This large cross section, and the effective transfer of the excitation energy of the 3p state to "seed" electrons via superelastic collisions was found to be a probable explanation of the very large ionization level obtained by McIlrath and Lucatorto (1976, 1977) in recent long-pulse-length laser experiments. While carrying out these calculations most of our two-electron model potential codes were also modified so that we can evaluate matrix elements involving continuum orbitals.

S. I. Chu (1978) has extended the method of Reinhardt (1976) and Chu and Reinhardt (1977) who carried out calculations for the intense field ionization of atomic hydrogen by circularly polarized radiation, employing a coordinate rotation transformation and L^2 - discretization of the atomic continuum.

Most of our effort has been directed towards constructing model potentials for the copper and zinc isoelectronic sequences. We have obtained accurate model potentials for Cu^+ , Zn^{+2} , Ga^{+3} and Ge^{+4} , and are in the process of calculating energy levels and transition probabilities for the one- and two-valence electron ions. Only the first four members of the copper isoelectronic sequence have been studied experimentally in sufficient detail so that accurate model potentials can be obtained.

4. Resonating States

We have published the results of configuration-interaction calculations of the non-relativistic eigenfunctions and eigenvalues of the $1s2p^2\ ^2P$ and $1s2p^2\ ^2D$ states of the lithium isoelectronic sequence (Fox and Dalgarno 1977) and we have calculated the radiative lifetimes of the $1s2p^2\ ^2P$ and 2D states. The values should be the most accurate available and they establish clearly that some of the measurements are erroneous.

5. Processes in Low Temperature Plasmas

We are continuing work on processes in low temperature plasmas. In our last proposal we mentioned work on scattering by polar molecules. That work was taken up by Dr. C. Bottcher and a description is now in press (Bottcher 1977).

6. Charge Transfer

We have completed our calculations of radiative charge transfer at thermal velocities (Butler, Guberman and Dalgarno 1977). We continue with non-radiative charge transfer. We have calculated the coupling terms for the case of N^{++} interacting with deuterium.

7. Laser Processes

We are exploring the atomic and molecular processes that determine energy transfer in gas lasers and we have begun with a study of the simple excimer Li_2 . We have calculated the transition dipole moments and we have shown that direct photodissociation is not possible. It appears that photodissociation occurs by discrete absorption into the $A^1\Sigma_u^+$ state followed by a transition into the $^3\Pi_u$ state which it crosses which is then succeeded by a transition into the $^3\Sigma_u^+$ state which dissociates. Because the process is initiated by line absorption the molecule is self-shielding.

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