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COHERENT EXCITATION OF AUTOIONIZING RESONANCES BY ELECTRON IMPACT

Progress Report

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N. L. S. Martin
Department of Physics and Astronomy
University of Kentucky
Lexington, KY 40506-0055

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N.L.S. Mart'n

Department of Physics and Astronomy, University of Kentucky
Lexington, Kentucky 40506-0055

Introduction

Experimental investigations have been carried out into interference effects caused by the coherent population, by electron impact, of cadmium autoionizing levels and continua of differing total angular momentum and parity. The work provides information on both the excitation mechanism by charged particle impact and the spectroscopy of autoionizing levels.

The experimental technique being used is electron-electron coincidence spectrometry. Differing binary and recoil peak intensities in coplanar $(e, 2e)$ ejected-electron angular distributions are caused by interference cross-terms, between opposite parity final-state continua, that change sign when $\theta_{ej} \rightarrow \theta_{ej} + 180°$ in the angular distributions.[1,2] The magnitude of these cross-terms varies rapidly with ejected-electron energy across overlapping autoionizing resonances. The energy variation in the interference terms may be isolated by obtaining the difference between $(e, 2e)$ energy spectra measured at ejected-electron angles 180° apart. Summation of the two spectra yields the dipole-allowed photo-electron spectrum.[3]

Experimental Work

The Position Sensitive Detection system installed last year is fully operational, and has enabled high quality, high resolution (~0.04eV) $(e, 2e)$ and non-coincident ejected-electron energy spectra to be obtained simultaneously. Of vital importance in the analysis of the data is the ability accurately to (intensity) normalize and (energy) align the pairs of $(e, 2)$ spectra taken 180° apart. This has been achieved using certain Auger peaks that appear in the non-coincident spectra; these peaks should have the same intensity and positions in the two spectra. This property has enabled the spectra to be aligned to better than 2 meV and normalized to better than 2%.

Experiments have been carried out for small momentum transfer $K \sim 0.2$ a.u. (small scattering angles); *i.e.* in the plane wave Born approximation (PWBA) limit. The momentum transfer axis may then be chosen as the quantization axis with the electron-impact excitation selection rule $\Delta M = 0$; the "parity favored" part of $(e, 2e)$ ejected-electron angular distributions are functions of the products of Legendre polynomials $P_J(\hat{k} \cdot \hat{K})$, where $\hat{k}$ is the ejected-electron direction. The spectral region investigated included the (well known) odd parity Cd $4d^9 5s^2 5p$ $J = 1$ and the (previously undetected) even parity Cd $5pnp$ $J = 0, 2$ ($n = 5, 6, 7$) autoionizing levels.

Three major experiments have been completed and a fourth is in progress. The experiments investigate different aspects of the interference effects by making use of the properties of Legendre polynomials.

1) For the "magic angle" between the ejected-electron directions and the momentum-transfer axis, $P_2(\hat{k} \cdot \hat{K})$ vanishes. The summed spectrum is thus the total (photoabsorption) cross-section. The difference spectrum contains only $(J = 1) \times (J = 0)$ interference; the fitted spectrum may be used in the analysis of experiment (2).

2) For ejected-electron directions along the momentum-transfer axis, all the Legendre Polynomials are unity. The summed spectrum is the "parity favored" partial cross-section ($^1P_1$ final state continuum). In the difference spectrum the $(J = 1) \times (J = 2)$ interference is a maximum; its contribution may be assessed after allowing for the $(J = 1) \times (J = 0)$ interference component obtained from experiment (1).

3) For ejected-electron directions perpendicular to the momentum-transfer axis, the summed spectrum is the "parity unfavored" partial cross-section ($^3P_1$ final state continuum). The difference spectrum provides a rigorous test of the *ab initio* calculation result that the $J = 0, 2$ autoionizing levels couple to the singlet, but not the triplet, continuum; *i.e.* the interference cross-terms should vanish.

4) (In progress) Experiments (1) and (2) correspond to the minimum and maximum $(J = 1) \times (J = 2)$ interference respectively. This experiment is being carried out for an intermediate ejected-electron direction which will provide a check on the quantitative analysis of the other experiments.

Theoretical Work

Up to the present time the experimental data have been compared with a calculation of the intereference effects that uses a number of approximations and assumptions. In particular, the magnitude of the interference terms has been left as a parameter to be fitted to the data. A series of *ab initio* calculations have recently been carried out in collaboration with M. Wilson .

1) HFR CI structure calculations for level positions and widths of Cd $4d^9 5s^2 5p +$ $5p6s + 5p7s + 5p8s + 5p5d$ $J = 1$ autoionizing levels. Recent work has shown that it is necessary to include the doubly excited states in order to obtain the correct dipole-allowed spectrum. [4]

2) HFR CI structure calculations for level positions and widths of Cd $5p^2 +$ $5p6p + 5p7p$ $J = 0, 2$ autoionizing levels. An accurate knowledge of these levels is important for the analysis of the interference effects.

3) Calculations of distorted wave phase shifts for the continuum electron in

$5sE\ell$ with $E = 0.01 \rightarrow 4.0$ eV and $\ell = 0 \rightarrow 3$. The results at low E are in excellent agreement with experimental $5sn\ell$ quantum defects.

4) PWBA amplitudes for the excitation of all the above autoionizing levels from the ground state. PWBA direct ionization amplitudes Cd $5s^2 \rightarrow 5sE\ell$ for $\ell = 0 \rightarrow 6$. These calculations will enable an absolute comparison of theory and experiment without recourse to normalization.

Discussion

A detailed comparison of experiment and theory is at present underway. A preliminary analysis suggests the following important conclusions.

1) The PWBA *magnitudes* appear to be of the right order to account for the observed interference effects. Whereas direct ionization due to the dipole term is negligible, the monopole and quadrupole terms are significant.

2) The relative *phases*, $\delta_{JJ'}$, of the PWBA amplitudes do not agree with the experimentally derived quantities. In order to obtain good agreement between experiment and theory it is necessary to include an extra phase $\approx -\pi/4$ in δ_{10}, and an extra phase $\approx +\pi/4$ in δ_{12}.

Both these findings are in qualitative agreement with the recent Coulomb-Born inner shell ionization calculations of Botero and Macek [*Phys.Rev.A* **45**, 154 (1992)], whose $(e, 2e)$ angular distributions required summation over several ℓ states. To the P.I.'s knowledge, experiment (1), described above, is the first experiment carried out under PWBA conditions that enables the extraction of the phase difference between the excitation amplitudes of only two ℓ states.

References

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Summary of Research Plans for 1994

The Cd experiments into the coherent excitation of $J = 0, 1, 2$ autoionizing levels and their associated continua will continue. In 1993 a number of $(e, 2e)$ experiments were carried out at small scattering angles in order to examine the validity of the plane wave Born approximation (PWBA) for small values of the momentum transfer K. Calculations of PWBA amplitudes were carried out, in a collaboration with M. Wilson, for all possible values of K. A detailed comparison of the experiments for small K and theory will be completed by the end of 1993. Preliminary analysis indicates that the PWBA *magnitudes* may be correct, but that their *phases* are in error by significant amounts. In 1994 the experiments will be repeated at larger scattering angles in order to examine the behavior of the excitation magnitudes and phases at larger K. The PWBA predicts that the magnitude of the dipole allowed $J = 1$ processes is proportional to $1/K$, and for the $J = 0, 2$ processes it is independent of K. Thus the dipole cross-section decreases as $1/K^2$, but the ratio of the interference cross-terms to the total cross-section is proportional to $(1/K)/(1/K^2) = K$. This indicates that although the absolute experimental count rates are expected to decrease fairly rapidly with increasing scattering angle, the relative interference effects will increase and should be readily observable. The PWBA calculations also predict that the direct ionization dipole process, which is negligible for $K \ll 1$ a.u., becomes significant as $K \to 1$ and should affect the observed Cd $4d^9 5s^2 5p$ $J = 1$ resonance line shape.

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