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The (e,2e) method for autoionization studies

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ABSTRACT - Present status and perspectives of further experiments on electron-impact excitation of atomic autoionizing states by the coincidence (e,2e) method are discussed on the basis of the current theoretical investigations in the Moscow-Dubna-Ulan-Bator group (Balashov, Grum-Grzhimailo, Lhagva, Magunov,Strakhova).

1. INTRODUCTION

It was more than twenty years ago when it was shown that the coincidence (e,2e) method can be of great use for autoionization studies [1]. This suggestion based on the unified theory of direct and resonance ionization of atoms by fast electrons [2] had another origin in nuclear physics where perspectives of similar coincidence experiments to investigate simultaneously two-step (via decaying states) and direct disintegration nuclear reactions drew much attention just at that time [3]. The pioneer (e,2e) experiments of the Flinders and Kaiserslautern groups [4,5] have demonstrated real advantages of the new method in physics of autoionization phenomena in atoms.

The theoretical analysis of the autoionization (e,2e) process presented here aims to stimulate further progress in the field.

2. COMMENTS ON RECENT EXPERIMENTS

2.1. Helium atom

The helium atom always played an extremely important role in the physics of autoionization phenomena as an excellent "laboratory" to develop and to test new many-body theoretical methods and models in this field. On the other hand, the main tendency in experimental investigation of helium autoionizing states using the coincidence (e,2e) method appears more to be a step by step improvement of the energy resolution in the ejected electron channel: Weigold et al. (1975) - 600 meV [4]; Pochat et al. (1982) - 350 meV [6]; Lower and Weigold (1990) - 150 meV [7]; McDonald and Crowe (1992) - 80 meV [8].

An objective is, in particular, to resolve the (2p^2)^1P and (2s2p)^1P states whose natural widths (72 and 38 meV) are only a little smaller than the separation energy of these two states (235 meV).

If resonances do not overlap then the triple differential (e,2e) cross section can be written as incoherent sum of individual
contributions from each resonance. The Fano and the Shore formulae may be used equivalently for this purpose [2]:

\[
\frac{d^3 \sigma}{d \Omega_s c d \Omega_e d E} = f_r(k_{ej}, Q) + \frac{1}{1 + \varepsilon_T^2} \sum_r a_r(k_{ej}, Q) b_r(k_{ej}, Q)
\]

\[1/\]

Generally, in the case of near lying resonances one has to sum amplitudes rather than probabilities corresponding to each of them:

\[
\frac{d^3 \sigma}{d \Omega_s c d \Omega_e d E} = \frac{k_f}{k_i} \left| T(k_{ej}, Q) \right|^2
\]

\[2/\]

In particular within the PWBA approach the total amplitude reads:

\[
T(k_{ej}, Q) = T_{direct}(k_{ej}, Q) + \sum_r T_r(k_{ej}, Q) \frac{q_r(Q) - 1}{\varepsilon_T + 1}
\]

\[3/\]

where \(q_r(Q)\) is the momentum transfer dependent Fano profile index for separate \(r\)-resonance. Note extended tails of each resonance profile represented by the formula above. Due to these tails resonance overlapping effects can be sensitive very much not only to the total energy resolution of experiment but also even to the instrumental profile. The problem of overlapping resonances is currently becoming increasingly important because of the progress of various auto-ionization studies and so precision electron impact experiments on the \((2p^2)^1D-(2s2p)^1P\) doublet in He are capital not only for the spectroscopy of helium atom itself but from this general point of view as well.

On fig.1 one can see noncoincidence ejected electron spectrum for the \((e,2e)\) process in helium measured several years ago by Oda et al. [9] with very high resolution at incident electron energies of \(1\) keV. Comparison between these data and recent PWBA calculations of double differential cross sections performed by Lhagva [10] by integrating the triple differential cross section /2/ over the scattered electron angles seems promising. Nevertheless it would be too hasty to propose such PWBA calculations for theoretical analysis of new and very interesting data for the \((e,2e)\) process on He at lower energies from the recent Flinders University [7] and Newcastle [8] coincidence experiments. The problem is that in the case of excitation the autoionizing \((2p^2)^3D\) state one must take into consideration on the same level two different mechanisms inducing the optically forbidden transition \((1s^2)^1S - (2p^2)^1D\). The first one is the one-step transition due to two - electron dynamical correlations in the atomic ground state; the other is a two-step excitation process via intermediate atomic states, here mainly via the level \((1s2p)^1P\). Preliminary calculations show a growing relative contribution of this multi-step process in the intermediate-energy region [11]. Our group is working now on an extention of the usual DWBA-approach to describe electron-impact multi-step excitation of autoionizing states in a way similar to that which had been used earlier for another problem [12].
2.2. Cadmium atom

(e,2e) experiments on Cd performed in 1980-1982 by Kevin Ross's group in Southampton with 150 eV electron beam [13,14] played a very important role in stimulating further developments in theory of the autoionization (e,2e) process. They clearly demonstrated that the PWBA approach had to give way to something more adequate to specific features of the process at intermediate energies. The DWBA went to the (e,2e) stage for the first time [15] in the context of autoionization.

At present these Southampton experiments find a fruitful continuation in Lexington [16,17]. The latest results obtained there by Nicolas Martin and his group put a lot of questions to the theory, among which the problem of interference between amplitudes of different multipolarities seems to be the most serious. Starting from the PWBA concepts the Lexinton group brought into use a number of specific procedures to collect data and to analyse it from the point of view of this problem. I mean, in particular, their procedure to sum ejected electron spectra measured for two opposite directions - parallel and antiparallel to the momentum transfer vector Q - to eliminate some interference effects. On the contrary, difference of such spectra gives the most evident information precisely about these effects.

Our theoretical group find many interesting problems connected with current experiments on Cd in Lexington. In the very near future we must estimate role of multi-step (two-step) transitions via intermediate states in excitation of positive parity levels such as 5p6p to have an unified picture of excitation of positive parity and negative parity states in the 4d-5p region. We see our task also in performing detailed DWBA calculations for various measured (e,2e)
characteristics in Cd to make theoretical analysis of them more realistic from the point of view of taking into account distortion and exchange effects.

In what follows rather good general agreement between theory and experiment will be shown concerning the \((e,2e)\) process in Cd. But one serious disagreement must be emphasised which remains unclear to us. Fig. 2 shows our DWBA calculations and Martin's data for ejected-electron \((e,2e)\) spectra in Cd summed for opposite ejection directions. The theoretical and experimental results are both given in arbitrary units but these units are the same for left and right sides of the picture. So, in spite of a good agreement between theory and experiment as it concerns the shape of the spectrum and its transformation with ejection angle, they disagree by about a factor of 2 in the ratio of total yields of ejected electrons in the two geometric variants of the experiment presented here. It is not obvious where the theory is going so seriously wrong, nor is it evident what steps should be taken to overcome this divergence.

![Fig. 2. Sum of \((e,2e)\) ejected-electron spectra in Cd [17]; curves – DWBA calculations from [18].](image)

3. THE DWBA FOR AUTOIONIZING STATES

Our theoretical investigations of distortion effects in the autoionization \((e,2e)\) process are made within the DWBA with exchange. Earlier we used this approach rather successfully when analyzing inelastic and superelastic electron scattering at intermediate energies [19]. Here, procedural aspects of the DWBA calculations will not be treated and the discussion will concern only the most pronounced transformations in the theory of the autoionization \((e,2e)\) process when going from the simplest PWBA approach to the DWBA. To my knowledge, the best paper demonstrating in detail general formalism of the DWBA theory for autoionization \((e,2e)\) process taking into account in a proper way interference between resonant (via autoionization state) and
direct (to continuum) ionization amplitudes is one given several years ago by Grum-Grzhimailo and Magunov [20] (unfortunately being published in Russian it remains quite unknown to the (e,2e) community).

According to the PWBA prescription the only m=0 sublevel with zero projection of angular momentum transfer on the Q-axis is populated. Violating the Q-axis symmetry distortion effects make it necessary to take into consideration a number of additional independent amplitudes of the (e,2e) process corresponding to different m values of the exited states. This leads to a reformulation of basic formulae of the resonance theory. In particular, the Fano profile index q appears in these formulae as a complex number.

In practice, one needs a lot of special information to make DWBA calculations consistent from point of view of using proper parameters in atomic wave functions and various interactions. Many additional experiments should be done to test optical potentials in the entrance and exit channels and final state interaction between an ejected electron and residual ion. So, experiments of direct (e,2e) process in vicinity of autoionizing states as well as traditional investigation of excitation of discrete atomic levels with the (e,e') and (e,e') methods turn out to be intimately linked with the (e,2e) autoionization program.

Theoretical description of autoionization (e,2e) experiments becomes much simpler in specific cases when only a small background of direct (e,2e) process takes place and so one can neglect interference between the resonant and direct amplitudes of the ionization process. Since the pioneer work by Southampton group [13] the cadmium atom attracted much attention just from this point of view. True, recent experiments by Martin et al. indicate that real situation with Cd is not so trivial. Nevertheless even now it seems to be a realistic first approach to formulate the (e,2e) theory for autoionizing states in this atom as an analog of that for the (e,e') process concerning discrete atomic levels.

Fig.3 shows our latest calculations [18] for differential cross-section of inelastic 150eV-electron scattering with excitation the 4d'5p:J=1(12.81eV) autoionizing state in cadmium performed within the DWBA with exchange. Contrary to our earlier paper [15] we used here intermediate-coupling atomic wave-functions [21] with Hartree-Fock orbitals together with an electron-atom optical potential constructed as static potential of the excited state and an effective local exchange potential corresponding to the electron cloud density in this excited state. These modifications move our previous calculations to better agreement with experiment. As for the angular correlation parameter ρ(θsc) (fig.4) the agreement is rather good up to about 20° but serious deviations appear for larger θsc.

4. ORIENTATION PARAMETERS OF AUTOIONIZING STATES

As the background of direct (e,2e) process into continuum in Cd in the region of the 4d'5p states is small, it is convenient to use the same polarization and alignment parameters to describe the spin-density matrix of the autoionizing states as those used traditionally for discrete atomic states in the (e,e') process. Fig.5 shows reduced statistical tensors A_{kq}=ρ_{kq}/ρ_{00} (in the collisional frame) for the autoionizing state 4d'5p:J=1 at 12.81 eV calculated within the DWBA with exchange. Due to a very small contribution of exchange scattering
Fig. 3. Differential cross section of excitation of the 4d\(^{-1}\)5p : J=1 (12.81 eV) autoionizing state in Cd by 150 eV electrons [14]; data - from ref. [14].

Fig. 4. The same as on fig. 3 but for the angular correlation parameter \(\beta(\theta_{sc})\) [18].

Fig. 5. Reduced statistical tensors \(A_{ij}(\theta_{sc})\) for autoionizing state 4d\(^{-1}\)5p : J=1 (12.81 eV) in Cd calculated within DWBA with exchange for incoming electron energy of 150 eV [18].

Fig. 6. Angular distribution of ejected electrons from the state 4d\(^{-1}\)5p : J=1 (12.81 eV) in Cd at 150 eV; PWBA and DWBA - calculations [18] for noncoplanar (e,2e) experiment.
amplitudes in the $e_{sc}$ region under consideration the orientation parameters as well as the shape of differential cross-sections are about the same for this state and for another J=1 state at 12.06 eV.

Various correlation characteristics of the autoionization $(e, 2e)$ process via these states including those related to spin polarization of ejected electrons (see part 5.3) can be formed from the set given in fig. 5 using standard formalism of angular momenta algebra \([22]\). In particular, the shift angle $\theta(e_{sc})$ giving position of the maximum in the coincidence ejected electron angular distribution is calculated as follows:

$$\tan \theta = -2 \rho_{21} \left[ \rho_{22} - \rho_{20} \sqrt{3/4} \right]^{-1}$$

5. ON SOME NEW $(e, 2e)$ EXPERIMENTS

I would like to discuss here from theoretical point of view perspectives to extend in some new directions experimental investigations of autoionizing states in the $(e, 2e)$ method.

5.1. Multichannel decay of autoionizing states.

Up to this point one class of atomic autoionizing states has been considered, namely, those lying between the first and the second ionization thresholds. The states above the second threshold are of great interest for many purposes. The $(e, 2e)$ experiments could give unique information concerning multichannel decay of such states.

Strakhova and coauthors have made a number of predictions for experiments on fast electron inelastic scattering on He with excitation of the series of autoionizing states converging to the n=3 ionization threshold [23]. Their calculations, performed taking into account the both internal and external configuration mixing, give a possibility to trace the variations in the branching ratio for the n=1 and n=2 decay channels dependent on the electron transfer momentum Q. The correctness of their predictions has been proved by similar calculations [24] of various characteristics of photoionization of the helium atom above the n=2 ionization threshold and performed using the same method to construct atomic wave functions for continuum and autoionizing states as was used for calculation of the electron impact ionization process. Among these characteristics one finds partial cross sections of ionization of helium to 1s, 2s and 2p states of the He$^+$ ion and the anisotropy parameter $\beta(n=2)$ in the angular distribution of ejected electron to the n=2 channel. One can think that the present-days multichannel theory of excitation of autoionizing resonances in He above the n=2 threshold can serve as a good guide for future $(e, 2e)$ experiments concerning the multichannel character of their decay. Note in connection with this suggestion that traditional $(e, 2e)$ experiments on direct ionization process on atoms and molecules now play more and more important role to investigate ionization channels to excited states of residual ions.

5.2. On noncomplanar $(e, 2e)$ experiments

Well-known $(p, 2p)$ experiments as well as other coincidence experiments in nuclear physics of this type have demonstrated serious advantages of coincidence measurements when performed not only in the complanar version but also out of the scattering plane. Recent $(e, 2e)$ experiments by Read et al. for direct ionization process in atoms show that this is also true for atomic physics.

We see the main objective of noncomplanar $(e, 2e)$ experiments with autoionizing states as getting more detailed information about mechanisms of their excitation and their decay properties. One knows
from general theoretical concepts that when coming down from the energy
region of applicability of the PWBA approach to intermediate energies
the angular correlation function of the two electrons in the \((e,2e)\)
process loses its axial symmetry relative the transfer momentum
direction \(Q=k_0-k_{e2}\). Qualitatively, the azimuthal asymmetry of the two
electron correlation function out the scattering plane and the symmetry
axis shift in this plane have the same origin in the distortion of
wave functions of incoming and of scattered electrons on excitation of the
atom. However, quantitatively, the magnitude of these two
distortion effects depends on different combinations of density matrix
elements (statistical tensors) of the states under consideration.

Fig. 6 illustrates our recent calculations of angular distribution of
the ejected electron over azimuthal angle \(\phi_{e1}\) in the \((e,2e)\) process
in Cd performed within the DWBA approach with exchange for incoming
electron energy of 150 eV. Detailed \((e,2e)\) measurements on decay of
autoionizing states out of the scattering plane are of great interest
from the point of view of the "complete experiment" aiming to get all
the parameters of the excitation process in a model independent way.

5.3. \((e,2e)\) with polarized electrons

Recent experimental and theoretical investigations of inelastic
(suprelastic) electron-atom scattering using polarized electron beams
(and, in some cases, polarized targets as well) open wide perspectives
to get detailed information concerning transition amplitudes between
discrete atomic levels. The same is expected to be true concerning
coincidence \((e,2e)\) experiments with polarized electrons for
autoionization transitions. Let us consider, as an example, electron
impact excitation of the \(2p^{-1}(3s^2):^2P\) autoionizing states in sodium
atom. Similarly to recent NIST experiment [25] on suprelastic electron
scattering when using a polarized electron beam and a polarized target
one could obtain a number of model independent parameters as
combinations of direct (nonexchange) and exchange amplitudes
corresponding to excitation of various sublevels of these autoionizing
states. Among them are the ratio of the cross sections for triplet and
inglet states of the total system Na-e and the angular momentum \(L\)
transferred to atom — separately for the states with definite total
spin of the incoming and atomic electrons. Coincidence \((e,2e)\)
measurements on decay of the autoionizing states could give important
additional information concerning the alignment angle \(\gamma\) of the charge
cloud in the excited atom.

Perhaps more difficult from a technical point of view but not less
informative could be coincidence \((e,2e)\) experiments with nonpolarized
incoming electrons to measure the spin polarization \(P_s\) of the ejected
electron. Fig. 5 contains all necessary data to calculate \(P_s\) for
electrons ejected from the autoionizing states \(4d^{-1}5p:J=1\) in Cd for any
genometry of a coincidence \((e,2e)\) experiment at 150 eV.

6. CONCLUSION

We have discussed here some aspects of the present status of the
coincidence \((e,2e)\) method in autoionization studies. No doubt, it has
good perspectives to be used and developed in further investigations of
mechanisms of excitation and decay of autoionizing states. It has been
shown also that many problems concerning the theoretical basis for
current and future experiments on this line remains to be solved. Our
group is continuing to work on many of them and we are interested very
much in closer collaboration with experimental groups which are working or are intending to work in the field.

I wish to take this opportunity of thanking the Organizing Committee (e,2e)'93 for their very important support given me to participate in the Symposium.

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