RESONANT ELECTRON SCATTERING BY METASTABE NITROGEN - revisited

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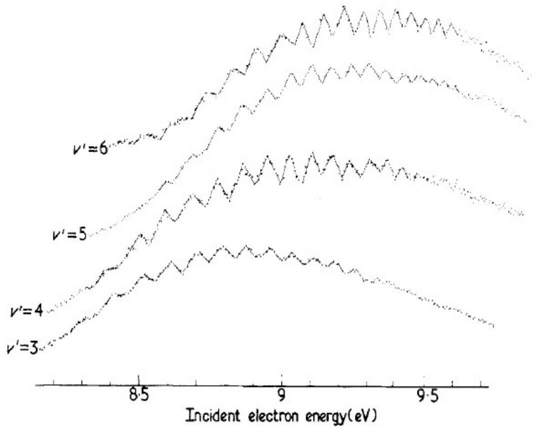
The intention of the present contribution is to renew attention to the resonant electron scattering by metastable $A^3\Sigma_u^+$ nitrogen involving the core excited shape resonance. This process was studied to some extent in the past but it is ignored in the recent modelling of the nitrogen plasma where it might be important.

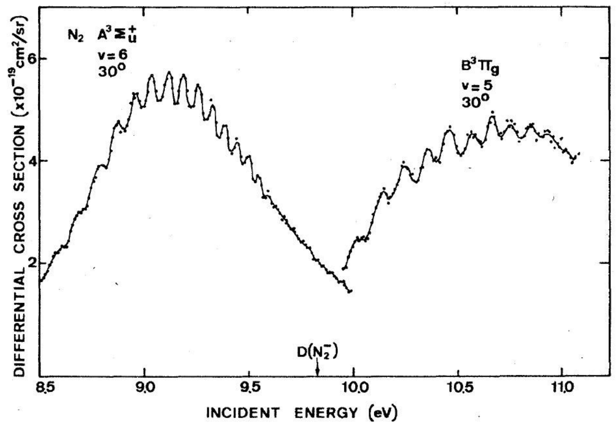
Resonant electron excitation of the $A^3\Sigma_u^+$ and $B^3\Pi_g$ states of nitrogen was experimentally studied by Mazeau et al. 1973 and later in more detail by the same Paris group, Huetz et al. 1980a, b, c.

Introduction – experimental evidence

Oscillatory structure in e-impact excitation functions of v=3 to 6 of $A^3\Sigma_u^+$ and v=1 to 5 of $B^3\Pi_g$ were observed by Mazeau et al. 1973 and confirmed by Huetz et al., 1980.



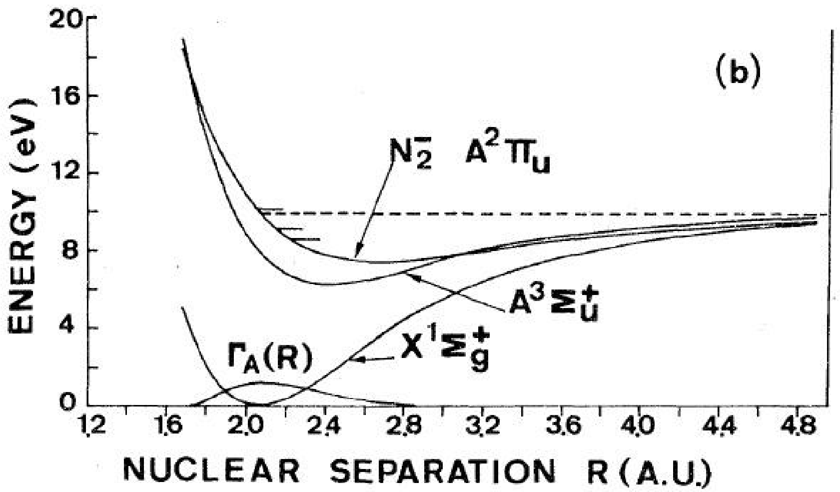
Mazeau et al. 1973



Huetz et al., 1980a

Observed structure, characteristic of the resonant scattering as well as angular distributions suggested resonant scattering through core-excited shape resonance of $^2\Pi_u$ symmetry.

$N_2(X^1\Sigma_g^+)+e \rightarrow N_2^-(A\,^2\Pi_u) \rightarrow N_2(A^3\Sigma_u^+)+e$



Core-excited resonance associated to the $A^3\Sigma_u^+$ parent state and having $^2\Pi_u$ symmetry was assumed to be involved in excitation of this state.

A classical local complex potential model was used to explain resonant oscillatory features observed in electron impact excitation of $A^3\Sigma_u^+$ first by Čadež and Fiquet-Fayard, 1973 and then, more extensively, by Huetz et al. 1980a, b, c.

The same model was used later by Čadež, 1983 to evaluate cross sections for the resonant electron impact excitation/de-excitation within the A-state vibrational manifold and for the resonant quenching of the $A^3\Sigma_u^+$ state to the $X^1\Sigma_g^+$ ground state.

Local complex potential LCP model

Local complex potential (LCP) model was initially developed in late 1960thies by Bardsley et al. 1966 and then used by Dubé L. and Herzenberg A., 1979 for resonant vibrational excitation (RVE) of N_2 and by Bardsley and Wadehra, 1979 for RVE of H_2. We have been applying LCP to discussing experimental RVE and dissociative electron attachment (DEA) using numerical programs developed by late Florance Fiquet-Fayard in 1973. LCP is recently extensively used by the Bari group of R. Celiberto (e.g. Laporta et al. 2014).

Florance Fiquet-Fayard

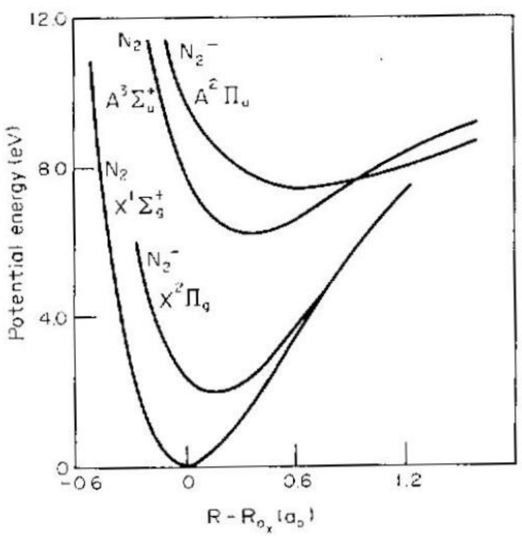
Key properties of the resonant state as described by LCP model are determined by nuclear wave-function of resonant complex which is solution of the nonhomogeneous Schrödinger equation with complex potential:

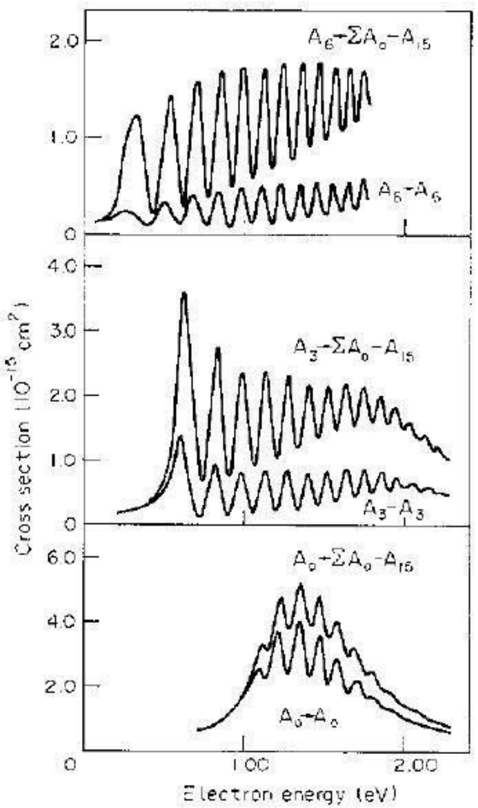
$$\left(-\frac{1}{2M}\frac{d^2}{dR^2}+\frac{J(J+1)}{2MR^2}+V^-(R)-\frac{i}{2}\Gamma(R)-E\right)\xi_J(R)=\frac{1}{\sqrt{2\pi}}\zeta_0(R)\chi_i(R)$$

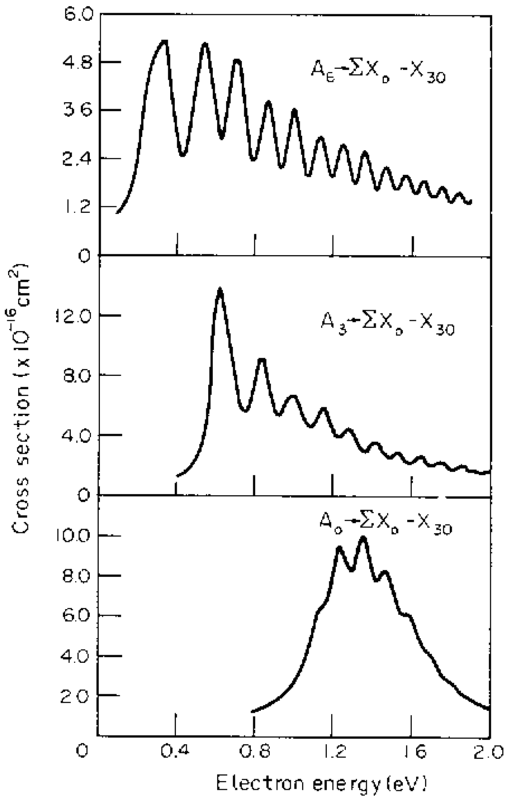
Cross section for RVE is obtained as a weighted overlap of resonant nuclear wave function and the final vibrational wave function of neutral molecule while cross section for DEA is determined from asymptotic behavior of resonant nuclear wave function when dissociation is energetically possible.

Resonant scattering by $N_2(A)$

LCP was used (Čadež, 1983) to evaluate cross sections for resonant electron scattering by N_2 ($A^3\Sigma_u^+$). The life-time of $A^3\Sigma_u^+$ state of N_2 is about 2s - electron collision can be considered as with a stable molecule. Calculation within LCP model was undertaken to evaluate potential importance of resonant electron impact reaction channel – big cross sections were obtained and thus potentially important for nitrogen plasma and discharge.







Čadež, 1983

Current status

Subsequent (after 1985) and present time literature challenge interpretation of experimental observations to being due to the core-excited resonant state of $^2\Pi_u$ and mainly ignores these experimental evidence.

- Characteristic resonant enhancement of v=6 excitation function $N_2(A^3\Sigma_u^+)$ was measured by Allan, 1989 but an alternative explanation of its origin as being possibly due to the low energy $^2\Pi_g$ resonance is mentioned.
- No evidence of possible $^2\Pi_u$ resonance was mentioned in *ab initio* calculations of electron impact excitation of triplet states in nitrogen by Gillan et al, 1996.
- The most detailed currently used data list on electron – nitrogen collision processes, Itikawa, 2006 does not comment on possible resonant excitation of the $N_2(A^3\Sigma_u^+)$.
- Resonant quenching of $N_2(A^3\Sigma_u^+)$ by electron impact is not considered in any present time plasma modelling.

Discussion and perspective

Low resolution differential excitation function for v=6 vibrational state of $A^3\Sigma_u^+$ at 30°, 60°,90° and 120° was re-measured by Paris group (Čadež et al, 1986).

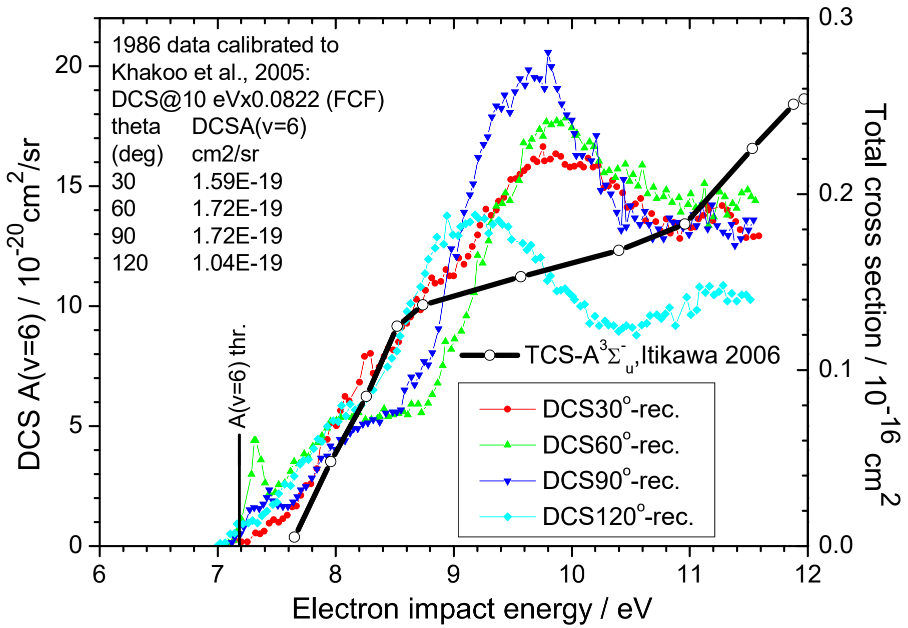


Figure: Data for relative A(v=6) DCS from Čadež et al, 1986 recalibrated to experimental absolute DCS at Ee=10eV of Khakoo et al., 2005 (left scale) and recommended total cross section (TCS) for excitation of N2(A) (right scale).

Resonant excitation of $A^3\Sigma_u^+$ apparently does not contribute noticeably to the TCS. This might be mainly due to its restricted energy and angular domain which diminish its visibility after summation over all vibrational states and integration over full scattering angle on the way to TCS.

However, the existence of a resonant excitation of $A^3\Sigma_u^+$ (and $B^3\Pi_g$) is doubtless and application of LCP was successful in description of RVE of A-state from ground (Huetz et al, 1980a) and excited (Huetz et al, 1980b) vibrational levels of $X^1\Sigma_g^+$ as well as of DEA to N_2 (Huetz et al, 1980c).

Discussion and perspective

The core-excited resonant state associated to N_2 $A^3\Sigma_u^+$ parent state (presumably of $^2\Pi_u$ symmetry) can have important role in understanding nitrogen plasma and discharge.

- Production of super elastic energetic electrons by resonant quenching of quasi stable $A^3\Sigma_u^+$. Importance of superelastic electron scattering is discussed by Laporta, 2017.
- Although the $A^3\Sigma_u^+$ state is the lowest triplet metastable state with long lifetime, the v=0 level of $B^3\Pi_g$ state has threshold just above v=6 of the A-state. As resonant features are observed in both states one can expect strong interference in resonant scattering process and thus more complex model is needed then it is simple LCP.
- Anionic molecular states play important role on surface processes. Lorente et al, 1999 have studied Auger type deexcitation of $A^3\Sigma_u^+$ by collision with metal surface. They find important influence of low energy $^2\Pi_g$ resonance. Core excited shape resonance might play important role in such process as well.

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