FIZIKA, 4 (1972) 157—163

INELASTIC e-H AND e-He COLLISIONS IN THE ADIABATICAL APPROXIMATION

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Received 23 December 1971; revised manuscript received 15 March 1972

Abstract: Using a diagonalized form of the interaction matrix in electron-atom scattering problem (adiabatic representation), some excitation and spin-change processes are calculated in e—H and e—He collisions. The configuration mixing of the diabatic states, allowing for the correlation effects in the system, is shown to be a significant factor in determining the near threshold behaviour of the inelastic cross section. The calculations demonstrate the superiority of the adiabatical representation in respect to the Born method even in the first order of the theory. The results are compared with the more elaborate calculations in the Veinshtein and close-coupling methods as well as with the experimental data.

1. Introduction

The possibility of applying the adiabatical approximation to the electron-atom scattering has been recently discussed by Smith[1] and Levin et al.[2]. The adiabatical representation of the direct and the exchange inelastic amplitudes for electron-atom collisions has been found recently by Janev and Ob'edkov[3–5]. There, the explicit form of the unitary transformation operator (which transforms the atomic-diabatic-basis to the adiabatical one) has been constructed in the framework of two-state approximation. The analysis of the obtained results shows that the configurational mixing, involved by the adiabatic representation, is significant for those diabatic states which energetically lie close one to another. This is the situation for electronic transitions between the excited states of the atom, and in particular for spin-change transitions. The ordinary methods of electron-atom excitation theory are either not applicable (Born-type methods), or very untractable (close-coupling method) in treating above mentioned inelastic processes.

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The aim of the present paper is to investigate the role of the configurational mixing of the diabatic states in the electron-atom excitation processes, especially in the energy region near the threshold, where this effect is expected to be significant. As illustrative examples we shall calculate the 1 s → 2 s, 2 p transition in hydrogen atom and the spin-change $1\,^1S \rightarrow 2\,^3S$, $2\,^3S \rightarrow 2\,^1P$ transitions in helium. Since the configurational mixing of the states is a correlation effect, we shall compare our results with the calculations where the correlations in the system are taken into account in some other way (e. g. close coupling method, Veinshtein approximation etc.). As our calculations are done in the first order of the perturbation theory, we shall also compare our results with the ordinary first order Born-type theories, based on the atomic wave function expansions (»diabatic« representation) to have a look about the convergence of the adiabatical perturbational series for the scattering amplitudes.

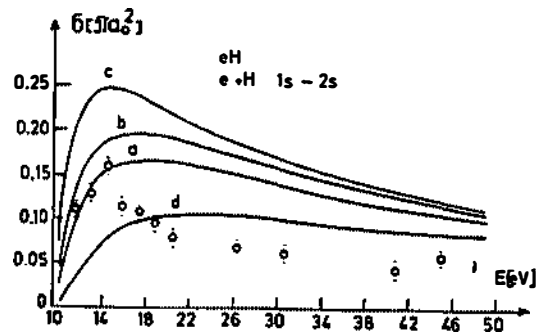

Fig. 1. e+H 1 s→2 s excitation. Curves *a* and *b* represent the results of adiabatical and quasi-adiabatical approximations, respectively. Curves *c* and *d* are the Born cross sections without and with exchange, respectively. The points are the experimental results of Stebbings et al.[6]

2. *Cross section calculations*

The explicit expressions for the direct and exchange inelastic amplitudes are given in Refs.[3,5]. We quote here the exchange amplitude for 1 → 2 transition

$$g(1 \rightarrow 2) = \frac{-2}{k^2} \int e^{i\vec{q}\vec{r}} X_2^*(\vec{r})\, X_1(\vec{r})\, d\vec{r} + O\left(\frac{1}{k^6}\right), \qquad (1)$$

where $\vec{k}$ is the incident electron momentum, $\vec{q}$ is the momentum transfer, X_1 and X_2 are the adiabatic wave functions, expressed in terms of the atomic wave functions φ_1 and φ_2 as

$$X_1 = \cos\alpha\,\varphi_1 - \sin\alpha\,\varphi_2,$$
$$X_2 = \sin\alpha\,\varphi_1 + \cos\alpha\,\varphi_2, \qquad (2)$$

where

$$\alpha = \frac{1}{2}\operatorname{arctg}\frac{2V_{21}}{V_{22}-V_{11}+\Delta E}, \qquad \Delta E = E_2 - E_1, \qquad (3)$$

or

$$\alpha' = \frac{1}{2}\operatorname{arctg}\frac{2V_{21}}{V_{22}-V_{11}}, \qquad V_{ik} = \langle\varphi_i|V|\varphi_k\rangle. \qquad (4)$$

The first choice of α we call adiabatical approximation, and the second one — quasiadiabatical.

In Ref.[3] was argued that, under some conditions, the direct amplitude f in the adiabatical representation is close to the direct Born amplitude. In the case of the transitions we intended to calculate, these conditions are fulfilled, so for f we shall take the first Born amplitude.

1 s → 2 s, 2 p excitation in e-H collisions. — The total excitation cross section for 1 s → 2 s, 2 p transitions in e-H collisions is calculated in standard way[6] using only for the exchange amplitude the adiabatical expression (1) with the two choices of α.

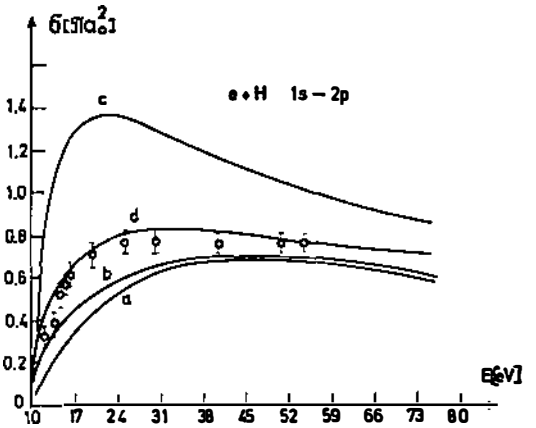

Fig. 2. e+H 1 s → 2 p excitation. Curves *a* and *b* — results of adiabatical and quasi-adiabatical approximations, resp. *c* — Born approximation without exchange; *d* — Veinshtein approximation. Experimental points are those of Fite et al.[5].

The results of calculations of 1 s → 2 s transition are shown in Fig. 1. The curve *a* is the adiabatical approximation and curve *b* is the quasiadiabatical

one. We see that in the threshold region and near the maximum of the cross section, both approximations give satisfactory agreement with the experimental data of Stebbings et al.[7]. In this region adiabatical approximation gives better results than the usual Born approximation (curves *c* and *d*; *c* — without exchange, *d* — with exchange). At higher energies the adiabatical approximation tends to Born results.

On Fig. 2 are represented the adiabatical calculations for 1 s → 2 p transition (curve *a* — adiabatical, curve *b* — quasiadiabatical). As in the previous case, the agreement of adiabatical results with the experimental data (Fite et al.[8]) is better than Born approximation (curve *c*). The curve *d* in this figure represents the calculations in Veinshtein approximation[9], which is a higher order approximation in respect to first order perturbational approximations.

Inelastic exchange e-He collisions. — The total excitation $i \to f$ cross section of helium atom is given by[10]

$$\sigma(i \to f) = \frac{8\pi}{k^2} \int_{q_{min}}^{q_{max}} \left(\frac{\lambda}{q^2} + \frac{\mu}{k^2}\right)^2 |\langle f | e^{i\vec{q}\vec{r}} | i \rangle|^2 q \, dq, \qquad (5)$$

where $|i\rangle$ and $|f\rangle$ are the initial and final state wave functions, and λ, μ are some constants. For transitions with the same multiplicity of the initial and

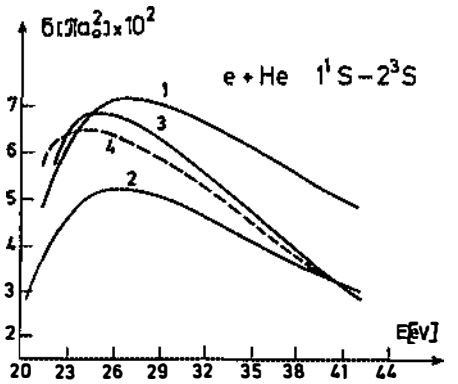

Fig. 3. e + He 1 ^{1}S → 2 ^{3}S excitation. Curve 1 is the result of quasiadiabatical approximation. Curves 2 and 3 are results of Born-Oppenheimer and Born-Ochkur approximations, resp. Curve 4 — experimental results of Gabriel and Heddle[11].

final states is $\lambda = -\mu = 1$. For the spin-change transitions $\lambda = 0$ and $\mu = \sqrt{3}$. In the last case we have

$$\sigma_{Sc}(i \to f) = \frac{1}{2\pi k^2} \int_{q_{min}}^{q_{max}} |g_{if}|^2 q \, d q \,. \tag{6}$$

We shall calculate the $1\,^1S \to 2\,^3S$ and $2\,^3S \to 2\,^1P$ transitions in He using for g the adiabatic expression (1). The atomic wave functions of the atomic electrons, entering in (2), we take from the papers of Veselov et al.[11] (for 1 s and 2 s states) and Burke et al.[12] (for 2 p states).

The results of $1\,^1S \to 2\,^3S$ calculations are given in Fig. 3. The curve 1 is the result of the quasiadiabatical approximation, using non-symmetrized atomic wave functions. The curves 2 and 3 are the calculations in the Born and Born-Ochkur[10] approximations, respectively. The dotted line 4 represents the experimental results of Gabriel and Heddle[13]. In this case the adiabatical results are satisfactory only in the threshold region. At higher energies the adiabatical results are worse even in respect to Born approximation, which might be a consequence of unsymmetrized wave functions used in our calculations.

In Fig. 4, the calculations of $2\,^3S \to 2\,^1P$ transition are given. Again, the curve 1 is the result of the quasiadiabatical approximation (the pure adiabatical result calculated with (r from (3) differs very little from the quasiadia-

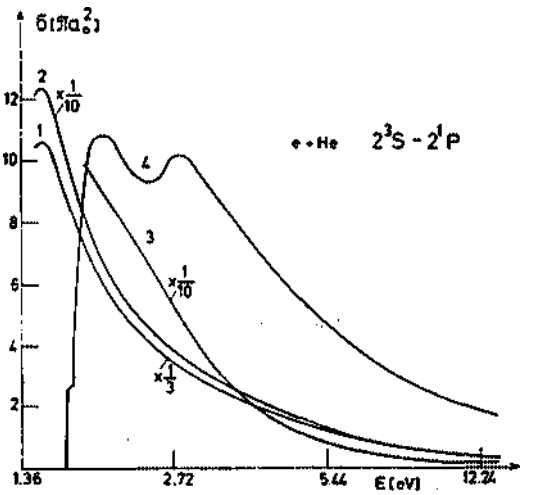

Fig. 4. e+He $2\,^3S \to 2\,^1P$ spin-change transition. Curve 1 — result of quasiadiabatical approximation, 2 and 3 are results of Born-Oppenheimer and Born-Ochkur approximations, respectively, 4 — close-coupling calculations of Burke et al.[12].

batical one) the curves 2 and 3 are the results in Born-Ochkur[14] approximations, respectively, and curve 4 represents the close-coupling calculations of Burke et al.[12].

In this case the results of the adiabatical approximation are much closer to the results of the most elaborate close-coupling method than the Born--Ochkur results, in the energy region above the cross section maximum. We note that the computational efforts needed in the adiabatical calculations are of the same order of magnitude as in the Born method and much less than those in close-coupling method.

3. *Conclusion*

Our calculations of some transitions in hydrogen and helium atoms show that the adiabatical mixing of the atomic states is an important mechanism governing the excitation and spin-change processes especially in the threshold region. This correlation effect in the scattering event acts parallely with some other factors such as virtual excitation of other reaction channels, polarization of atomic orbitals etc., which are subject of description of some more elaborated methods of electron-atom scattering theory. This fact enables one to construct such an adiabatical representation in which other correlation effects can be superposed to the adiabatical mixing of the states.

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NEELASTIČNI e-H I e-He SUDARI U ADIJABATSKOJ APROKSIMACIJI

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Sadržaj

Koristeći jednu dijagonaliziranu formu matrice interakcije za elektron--atomski problem rasejanja (tzv. adijabatska reprezentacija), neki eksitacioni i spin-izmenski procesi su izračunati za e-H i e-He sudare. Pokazano je da mešanje konfiguracija atomskog bazisa predstavlja značajan korelacioni efekt koji određuje ponašanje preseka neelastičnog procesa u blizini praga.

Ova konkretna izračunavanja nekih neelastičnih procesa pokazuju superiornost adijabatske reprezentacije u odnosu na Bornov metod još u prvom redu perturbacione teorije.

Rezultati se upoređuju s izračunavanjima u drugim aproksimacijama koje uzimaju u obzir korelacione efekte (Vajnštajnov metod, metod jake sprege) i sa eksperimentalnim podacima.