increase of the threshold pump powers, and to a decrease of the gain. We are now planning experiments aimed at determining the requirements that the monochromaticity of the pump radiation must satisfy to obtain optical amplifiers and laser-frequency convertors.

The authors thank S. G. Przhibel'skiĭ for valuable theoretical consultations and A. M. Bonch-Bruevich for interest in the work.

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1)See also [13] on this subject.

[1] S. G. Rautian and I. I. Sobel'man, Zh. Eksp. Teor. Fiz. 41, 456 (1961); 44, 934 [Sov. Phys. JETP 14, 328 (1962); 17, 635 (1963)].
[2] P. A. Apanasevich, Opt. Spektrosk. 14, 612 (1963); 16, 709 (1964).
[3] T. I. Kuznetsova and S. G. Rautian, Zh. Eksp. Teor. Fiz. 49, 1605 (1965) [Sov. Phys. JETP 22, 1098 (1966)].
[4] S. G. Rautian, in: Nelineĭnaya optika (Nonlinear Optics) Nauka, 1968, p. 3.
[5] P. A. Apanasevich, Dokl. Akad. Nauk BSSR 12, 878 (1968).
[6] D. F. Smirnov and A. S. Troshin, Vestn. Leningr. Univ. 4, No. 1, 93 (1971).
[7] B. R. Mollow, Phys. Rev. A 12, 1919 (1975); 188, 1969 (1969).
[8] F. Shuda, C. Stroud, and M. Hercher, J. Phys. B 7, L 198 (1974).
[9] W. Hartig, W. Rasmussen, and H. Walter, Z. Phys. A 278, 205 (1976).
[10] A. M. Bonch-Bruevich, V. A. Khodovoĭ, and N. A. Chigir', Zh. Eksp. Teor. Fiz. 67, 2069 (1974) [40, 1027 (1975)].
[11] A. M. Bonch-Bruevich, S. G. Przhibel'skiĭ, V. A. Khodovoĭ, and N. A. Chigir', Zh. Eksp. Teor. Fiz. 70, 445 (1976) [Sov. Phys. JETP 43, 230 (1976)].
[12] R. Tanas and S. Kielich, Opt. Commun. 14, 173 (1975).
[13] J. M. Winter, Ann. Phys. (N.Y.) 4, 745 (1959).
[14] A. Mitchell and M. Zemansky, Resonant Radiation and Excited Atoms, McMillan, 1935.
[15] É. M. Anderson and V. A. Zilitis, Opt. Spektrosk. 16, 177 (1964).

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Dissociative recombination of electrons on the molecular ions H_2^+ and D_2^+ with production of strongly excited atoms

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The process of dissociative recombination with production of strongly excited atoms in collisions between electrons of energy 1–13 eV and molecular ions is considered. The recombination cross sections are calculated for the system $e+H_2^+$ (D_2^+) with formation of excited atoms in states with $n \geq 3$ for different vibrational states of H_2^+ (D_2^+). The calculation results are compared with the available experimental measurements. The transition from the quantum description of the motion of the nuclei in dissociative recombination to the classical description is indicated.

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1. INTRODUCTION

One of the important elementary processes that lead to the decay of the electron density in recombining discharges and to the vanishing of electrons and ions from the upper layers of the atmosphere is the dissociative recombination (DR) process

$$e+AB^+ \to AB^* \to A+B^*,$$

in which collision of the electron with the molecular ion produces an autoionization state AB^* with a repulsion term, nuclear motion over which leads to formation of recombination products.

The rate coefficients of DR at thermal energies of the electrons were measured in recombining discharges for many ions (see the reviews[1,2]). For the simplest ions H_2^+ and D_2^+ there was no experimental information on the DR cross sections until recently, because of the rapid formation of the H_3^+ (D_3^+) and H_5^+ (D_5^+) at relatively high pressures of the recombining discharges. Only in recent experiments with crossed beams[3-5] were DR cross sections measured at relative energies on the order of several electron volts, namely, the total DR cross section for collisions with H_2^+ and D_2^+ was measured at energies 0.6—7 eV, in[3] and the DR cross section with production of $D(n=4)$ was measured at energies 1.4—7.5 eV, in[4] and the cross section for recombination with production of $D(n=2)$ was measured at energies 1.4—7.5 eV in[5].

The theoretical papers[6-9] devoted to the description of DR in collisions with H_2^+ and D_2^+ are restricted mainly to slow (up to 1 eV) electrons and to the case when the repulsion term of the autoionization state crosses the ground vibrational state of the molecular ion. The results of these studies cannot be used to describe DR with production of strongly excited ($n \geqslant 3$) states of hydrogen or deuterium. Thus, the first estimates of the DR cross sections for the system $e+H_2^+$ and energies < 1 eV via production of the autoionization states $H_2^*(2p\sigma_u, 2s\sigma_g, {}^3\Sigma_u)$ and $H_2^*(2p\sigma_u, 2p\pi_u, {}^3\Pi_g)$ were carried out by Bauer and Wu[6] and were repeated with slight modifications by

Wilkins.[7] Dubrovskiĭ and Ob"edkov[8] have considered DR at energies < 5 eV via the $(2p\sigma_u)^2\,{}^1\Sigma_g$ state. A cycle of papers by Nielsen *et al.*[9] is devoted to DR of thermal electrons in collisions with strongly vibrationally or rotationally excited H_2^+ ions via direct transfer of the electron energy to the nuclear motion (violation of the Born-Oppenheimer approximation).

In the present paper, using collisions with H_2^+ and D_2^+ ions as example, we consider DR with production of strongly excited atoms (we use the atomic system of units).

2. FUNDAMENTAL FORMULAS

Dissociative recombination of an electron colliding with H_2^+ (or D_2^+), in the case of interest to us

$$e+H_2^+\rightarrow H(1s)+H^*(n,\ l),\quad n\geqslant 3, \tag{1}$$

proceeds as a result of excitation of the electron from the ground $1s\sigma_g$ state to the $2p\sigma_u$ state with simultaneous capture of the incident electron into a Rydberg state with quantum numbers $n, l, m (n\geqslant 3)$. The behavior of the term of the produced autoionization state is determined by the binding energy of the $2p\sigma_u$ electron and is repulsive (Fig. 1). The decay times of the autoionization states with $n\geqslant 3$ (see Fig. 2) exceed the nuclear dispersal time (~ 10^{-15} sec), so that practically each act of formation of the autoionization state is accompanied by dissociation of the molecular ion.

The nuclei move slowly in comparison with the electrons, and hardly change their position during the collision time. Therefore the capture cross section can be calculated at a fixed position of the nuclei, and the resultant expression can then be averaged over the motion of the nuclei. The cross section for the production of the autoionization state (n,l,m) in scattering of monokinetic electrons with quantum numbers $(E,l',0)$ are determined by the Breit-Wigner formulas[10]

$$\sigma_{nlm,El'0}(\mathrm{R})=\frac{(2l'+1)\pi\Gamma_{nlm,El'0}(\mathrm{R})\Gamma_{nlm}(R)}{k^2[(E-u_{if}(R))^2+{}^1/_4\Gamma^2_{nlm}(R)]}, \tag{2}$$

where $k^2/2=E$ is the energy of the incident electron, $\Gamma_{nlm,El'0}$ and Γ_{nlm} are the elastic and total decay widths of the autoionization state (n,l,m); $u_{if}(R)=E_{nlm}(R)-E_g(R)$, $E_{nlm}(R)$ is the term of the autoionization state, and $E_g(R)$ is the term of the ground state of H_2^+ or D_2^+. Multiplying (2) by the square of the radial nuclear wave function and integrating with respect to dR, we obtain

$$\sigma_{nlm,El'0}(\mathrm{R}_E)=\frac{(2l'+1)2\pi^2F_v^2(R_E)\Gamma_{nlm,El'0}(\mathrm{R}_E)}{k^2|du_{if}(R_E)/dR|}, \tag{3}$$

where v is the vibrational quantum number, R_E is the internuclear distance at which capture of electrons with energy E is most probable and is determined from the condition

$$E_{nlm}(R_E)-E_g(R_E)=E. \tag{4}$$

Expression (3) must be summed over l' and averaged over all the directions of the internuclear axis (i.e., over the directions of R_E) relative to the electron-incidence direction. The last operation cannot be carried out in general form, and we therefore describe a concrete method of calculating the decay widths of the autoionization states.

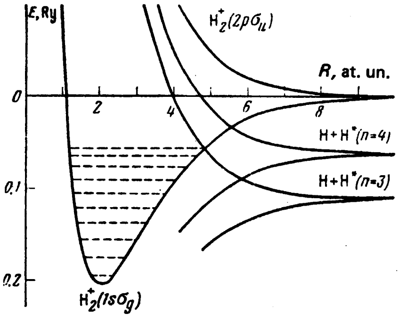

FIG. 1. Diabatic potential curves of the system $H+H^*(n\geqslant 3)$.

The dimension of the "orbit" of the strongly excited $(n\geqslant 3)$ electron in the autoionization state $H_2^*(2p\sigma_u, nlm)$ greatly exceeds the dimension of the molecular ion H_2^+. Therefore the behavior of the wave function of a strongly excited electron is determined mainly by the Coulomb field of the molecular ion $H_2^+(2p\sigma_u)$, and the wave function of the autoionization states can be chosen with good approximation in the form

$$\Psi_{u,nlm}=\Phi_u(\mathbf{r}_1,\mathbf{R})\Phi_{nlm}(\mathbf{r}_2),\quad \Phi_{nlm}=\frac{\varphi_{nl}(r_2)}{r_2}Y_{lm}(\mathbf{r}_2), \tag{5}$$

where Φ_u is the wave function of the $2p\sigma_u$ state of the electron in the H_2^+ ion, and Φ_{nlm} are the Coulomb hydrogen functions quantized for the direction of motion of the incident electron. The wave function of the continuous spectrum takes in this approximation the form

$$\Psi_{g,El0}=\Phi_g(\mathbf{r}_1,\mathbf{R})\Phi_{El0}(\mathbf{r}_2),\quad \Phi_{El0}=\frac{\varphi_{El}(r_2)}{r_2}Y_{l0}(\mathbf{r}_2); \tag{6}$$

here Φ_g is the wave function of the $1s\sigma_g$ state in the H_2^+ ion; φ_{El} is the Coulomb hydrogen radial wave function of the continuous spectrum normalized in energy and having an asymptotic form

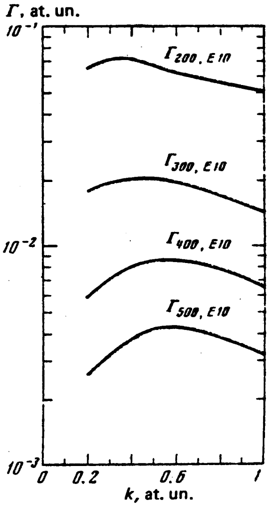

FIG. 2. Decay widths (10a) for the 2*s*, 3*s*, 4*s*, and 5*s* states. The internuclear distance at which decay at a given energy takes place is determined by condition (4).

$$\varphi_{El}(r) \xrightarrow[r\to\infty]{} \left(\frac{2}{\pi k}\right)^{1/2} \sin\left(kr+\frac{\ln 2kr}{k}-\frac{\pi l}{2}+\delta_l\right).$$

The exchange effects are disregarded since they are numerically smaller.

The diabatic potential curves of the autoionization states (see Fig. 1) take in this approximation the form

$$E_{nlm}(R)\approx E_u(R)-1/2n^2. \tag{7}$$

Exact numerical calculations of the terms $E_{g,u}(R)$ for H_2^+ were taken from.[11] In accordance with (7), the function $|du_{if}(R)/dR|$ for all the autoionization states with $n\geq 3$ is approximately the same:

$$\frac{du_{if}(R)}{dR}\approx\frac{d}{dR}(E_u(R)-E_g(R)) \tag{8}$$

and was obtained from the data given in.[11]

The electron of the molecular ion is more strongly bound in the initial and final states than the incident electron captured into a strongly excited state. In the calculation of the decay widths we therefore confine ourselves to the dipole-dipole term $(\mathbf{r}_1\circ\mathbf{r}_2)/r_2^3$ of the expansion of the interelectron interaction in the negative powers of r_2

$$\Gamma_{nlm,El'0}(\mathbf{R}_E)=2\pi|\langle\Psi_{u,nlm}\left|\frac{1}{r_{12}}\right|\Psi_{g,El0}\rangle|^2$$

$$\approx 2\pi d^2(R_E)\left(\frac{k^2}{2}+\frac{1}{2n^2}\right)^4|\langle\Phi_{nlm}(\mathbf{r}_2)\left|\frac{(\mathbf{R}_E\mathbf{r}_2)}{R_E}\right|\Phi_{El0}(\mathbf{r}_2)\rangle|^2. \tag{9}$$

The dipole moment $|d(R)|=|\langle\Phi_g(r,R)|r|\Phi_u(r,R)\rangle|$ is tabulated in [12]. This method of calculating the decay width corresponds in the theory of ion excitation by electron impact to the Van Regemorter approximation.[13]

In accordance with the selection rules for the dipole transitions, it follows from (9) that when electrons with quantum numbers $(el0)$ are scattered, the main result is excitation of autoionization states with $\Delta l=\pm 1, m=0, \pm 1$. Using the well known rules[14] for the calculation of the dipole matrix elements, we obtain after averaging over the directions of the internuclear axis

$$\Gamma_{nl0,El'0}(R_E)=\frac{2\pi d^2(R_E)l_{max}^2}{3(4l_{max}^2-1)}\left(\frac{k^2}{2}+\frac{1}{2n^2}\right)^4M_{nl,El'}^2,$$
$$l_{max}=\max(l,l'); \tag{10a}$$

$$\Gamma_{n(l+1)\pm1,El0}(R_E)=\frac{\pi d^2(R_E)(l+1)(l+2)}{3(2l+3)(2l+1)}\left(\frac{k^2}{2}+\frac{1}{2n^2}\right)^4M_{nl+1,El}^2, \tag{10b}$$

$$\Gamma_{n(l-1)\pm1,El0}(R_E)=\frac{\pi d^2(R_E)(l-1)l}{3(4l^2-1)}\left(\frac{k^2}{2}+\frac{1}{2n^2}\right)^4M_{nl-1,El}^2. \tag{10c}$$

The matrix elements $M_{ll'}$ are tabulated in[15]:

$$M_{ll'}=\int_0^\infty\varphi_{nl}(r)\varphi_{El'}(r)r\,dr.$$

The characteristic behavior of the decay widths is illustrated in Fig. 2. The cross section of DR with production of hydrogen atoms in the states (nl) is determined in accordance with (3) and (10) by the expression

$$\sigma_{nl,E}=\sum_{ml'}\sigma_{nlm,El'0}$$

$$=\frac{4\pi^3d^2(R_E)F_v^2(R_E)}{3k^2|du_{if}(R_E)/dR|}\left(\frac{k^2}{2}+\frac{1}{2n^2}\right)^4(lM_{nl,El-1}^2+(l+1)M_{nl,El+1}^2). \tag{11}$$

The cross sections $\sigma_{nl,E}$ are proportional to the cross sections for the photoionization of the excited states of the hydrogen atom.

The total recombination cross section on a level with given quantum number n is equal to

$$\sigma_{n,E}=\sum_l\sigma_{nl,E}. \tag{12}$$

The quantum analysis of the nuclear motion, which is given in the Appendix shows that in order for (11) to be valid it suffices that the radial motion of the nuclei be quasiclassical, and the square of the radial wave function $F_v^2(R_E)$ must be averaged over the oscillations. We, however, will use formula (11) for the description of the DR of all the vibrational states.

The diabatic term of the repulsion autoionization state $H_2^*(2p\sigma_u, nl)$ crosses the Coulomb condensation of the binding diabatic states $H_2^*(1s\sigma_g, n'l')$ with $n'>n$. The term splitting at the crossing points can be calculated by a method analogous to the calculation of the widths. The calculations show that in the case when the decay widths are small in comparison with the time of dispersal of the nuclei and the decay of the autoionization states can be disregarded, the values of the term splittings are also small. We therefore disregard the non-diabatic transitions between the terms.

At interatomic distances $R>35$ *at. un.*, the diabatic potential curves of the states $H^*(n\geq 3)+H$ cross a term of the system $H^+ + H^-$. The exchange interaction at such distances is small[16] ($<2\times 10^{-2}$ eV) and the non-diabatic transitions can also be disregarded in this case at electron-volt energies of the dissociation products.

3. RESULTS OF CALCULATIONS AND DISCUSSION

The calculated cross sections for the DR of electrons with energy 1—13 eV on H_2^+ and D_2^+ ions followed by production of excited atoms with $n=3$ and 4 are shown in Figs. 3a—3d. With increasing relative energy, the cross sections decrease rapidly (faster than $1/k^2$). According to (11), at a given n, the distribution over l is determined only by the electron energy and does not depend on the vibrational quantum number and consequently on the isotopic modification. The distribution with respect to l for $n=3$ and 4, as a function of the electron energy, is given in Table I.

The DR cross sections (11), as already noted, are proportional to the photoionization cross sections of the excited states of the hydrogen atom. To calculate the photoionization cross sections of strongly excited states at electron energies <13 eV we can use the Kramers formula,[14] according to which the average photoionization cross section of one of the $\sim n^2$ states with practical quantum number n is proportional to $1/n^5$. The dissociation cross section (12) is proportional to the product

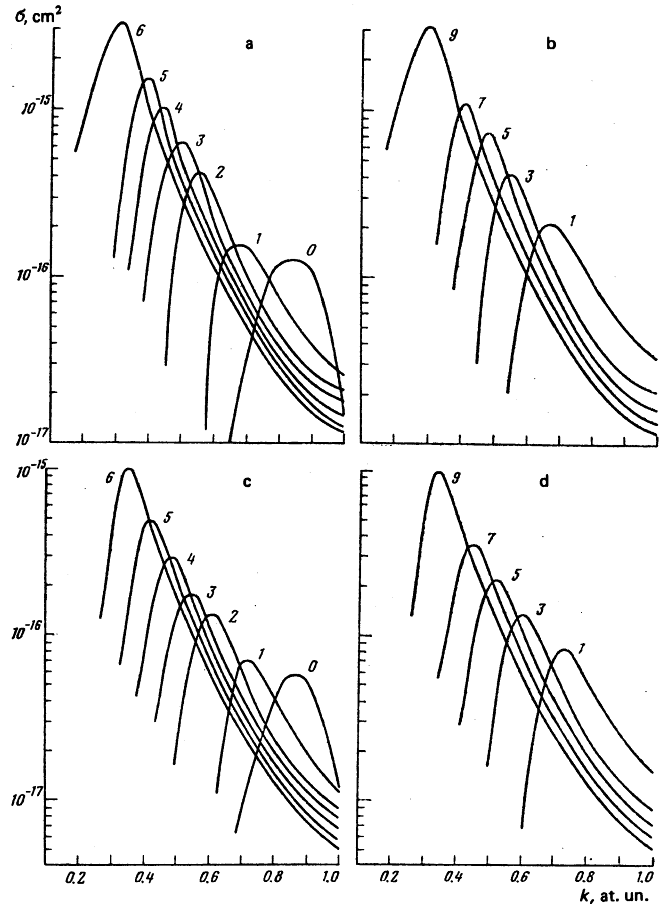

FIG. 3. Cross sections of dissociative recombination in collisions of electrons with H_2^+ or D_2^+ with production of a—$H^*(n=3)$, b—$D^*(n=3)$, c—$H^*(n=4)$, d—$D^*(n=4)$. The labels on the curves are the vibrational quantum numbers of the ion.

of the average photoionization cross section by the total number of states, i.e., $\propto 1/n^3$. This relation is already well satisfied for $n=4$ and 5. Therefore the cross section for dissociation with production of atoms with $n>4$ takes the form

$$\sigma_{n,E} \approx (4/n)^3 \sigma_{4,E}. \tag{13}$$

It should be noted that the Kramers approximation provides a good picture, on the average, i.e., for the cross sections (13) of dissociation with production of atoms with definite principal quantum number. It is seen seen from Table I that the dissociation proceeeds mainly with production of small angular momenta. Thus rule holds also for dissociative recombination with production of more strongly excited states with $n>4$. It is precisely the small angular momenta which determine the proportionality to $1/n^3$ in formula (13).

TABLE I. Distribution % with respect to the angular momenta for DR with production of excited H or D atoms with $n=3$ and 4.

Electron states	k, at. un.								
	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1
3*s*	16.8	20.8	25.7	31.2	37.0	42.2	48.0	52.2	57.0
3*p*	45.1	48.3	50.4	51.0	49.7	47.5	44.3	42.0	38.6
3*d*	38.1	30.9	23.9	17.8	13.3	10.3	7.7	5.8	4.4
4*s*	11.9	16.3	21.3	27.6	33.5	39.5	45.0	50.4	54.7
4*p*	33.3	39.6	45.0	46.8	47.3	46.2	44.2	41.5	38.9
4*d*	37.6	33.7	28.1	22.3	17.3	13.2	10.1	7.7	6.1
4*f*	17.2	10.4	5.6	3.3	1.9	1.1	0.7	0.4	0.3

In the experiment of[3-5], the H_2^+ or D_2^+ ionbeams were obtained by ionizing molecular hydrogen or deuterium with fast electrons. The vibrational-state distribution of the resultant ions does not depend in this case on the energy of the ionizing electrons and is approximately proportional to the Franck-Condon factors (the squares of the overlap integrals) between the vibrational nuclear wave function of the ground state of H_2 (or D_2) and the wave functions of the vibrational states of H_2^+ (or D_2^+). The exact distribution over the vibrational states of H_2^+ and D_2^+ was measured in an experiment[17] on the photodissociation of the molecular ions H_2^+ and D_2^+ and is given in Table II.

Figure 4 shows the cross sections for dissociation with production of atoms with $n=3$ and 4, calculated with account taken of the experimentally measured distribution over the vibrational states of the H_2^+ and D_2^+ ions. Vibrational states with $v \leqslant 6$ for H_2^+ and with $v>9$ for D_2^+ were taken into account. The contributions of the vibrational states with $v>6$ for H_2 and $v>9$ for D_2^+ respectively were added to the contributions of the vibrational states with $v=6$ and 9. The figure shows also the cross section for recombination to all levels with $n \geqslant 3$. The contribution to the recombination of the levels with $n>4$ was calculated from formula (13). Estimates of the decay widths in the recombination to $n=2$ by formulas (10) yield (see Fig. 2) a value ~2 eV, corresponding to decay times $\sim 4 \times 16^{-16}$ sec. The nuclei cannot manage to move apart during this time, so that we can assume that recombination to the $n=2$ level does not make a noticeable contribution to the total recombination cross section, as is confirmed by experiment[5] (see Fig. 4b). Therefore the cross section for recombination to levels with $n \geqslant 3$ should be close to the total recombination cross section.

The calculated recombination cross section to levels with $n \geqslant 3$ (see Fig. 4) is approximately 1—1.5 times larger than the measured[3] total recombination cross section.

The recombination cross sections to the level $n=4$ of electrons with D_4^+ were measured[4] under two assumptions: a) that only the *s* state is populated; b) that all the angular momenta are simultaneously populated. Our theory gives an intermediate position (Table I, the *s* and *p* states are predominantly populated), therefore the results of our calculations are compared in Fig. 4 with the arithmetic mean of the experimental cross sections obtained under the assumptions made above. Assuming the same energy dependence, the calculated cross section is approximately double the measured value.

TABLE II. Distribution % over the vibrational levels obtained upon ionization by fast electrons [17].

	v										
	0	1	2	3	4	5	6	7	8	9	$\Sigma v>9$
H_2^+	11.9	19.0	18.8	15.2	12.5	7.5	5.2	3.7	2.4	1.6	2.2
D_2^+	4.5	10.4	14.1	14.8	13.4	11.1	8.5	6.3	4.2	3.4	9.3

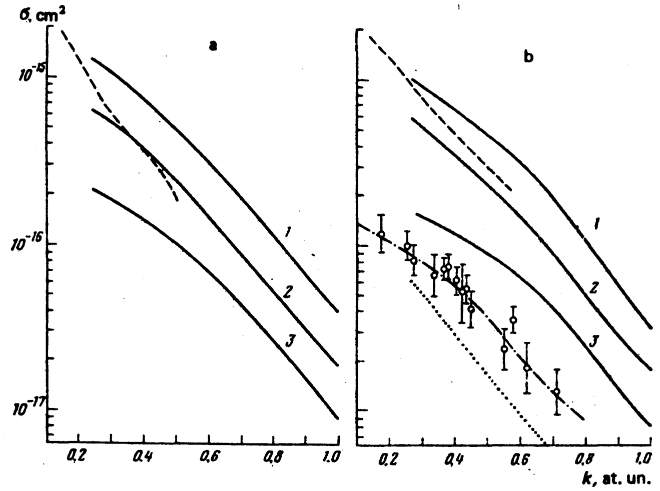

FIG. 4. Cross sections of dissociative recombination $e+H_2^+$ (D_2^+) with account taken of the distribution over the vibrational levels,[17] obtained upon ionization of $H_2(D_2)$ by fast electrons. a—$e+H_2^+$, dashed—experimental [3] total DR cross section, solid—our calculation: 1—total cross section of DR to levels $n \geqslant 3$, 2—cross section of DR with production of $H^*(n=3)$, 3—with production of $H^*(n=4)$. b—$e+D_2^+$, dashed—experimental [3] total DR cross section, dash-dot and individual points—experimental[15] DR cross section with production of $D^*(n=4)$, dotted curve—experimental [5] cross section of DR with production of $D^*(n=2)$. Solid lines—our calculation: 1—to all levels with $n \geqslant 3$, 2—with production of $D^*(n=3)$, 3—with production of D^* $(n=4)$.

4. CONCLUSION

In the present calculations of the DR we used three approximations: 1) the radial motion of the nuclei was assumed quasiclassical; 2) the wave functions of a strongly excited electron and of an electron with a continuous spectrum were taken in pure Coulomb form; 3) we used the dipole-dipole approximation to calculate the decay widths. Comparison with the experimental measurements shows that within the framework of these approximations we can account for the main regularities of the DR with production of strongly excited atoms.

APPENDIX

A large number of formulas similar to (3) and valid for quasiclassical motion of the nuclei have been obtained in the literature, from qualitative considerations, for the description of DR (see, e.g.,[1,2,6,7]. However, the direct transition from the quantum motion of the nuclei to the classical motion was nowhere considered. In this Appendix we trace this transition and show that in dipole-dipole interaction of the electron formula (3) is valid under a more general condition, namely, it suffices only that the radial motion of the nuclei be quasiclassical.

For the sake of argument we consider the transition of an incident electron with quantum numbers $(n, l'=l+1, 0)$ to an excited state $(n, l, 0)$. At other relations between l' and l, the analysis is similar. Formula (3) with (10a) taken into account yields in this case

$$\sigma_{nl0,E(l+1)0}=\frac{4\pi^3 d^2(R_E)F_v^2(R_E)\,(l+1)^2}{3k^2|du_{if}(R_E)/dR|\,(2l+1)}\left(\frac{k^2}{2}+\frac{1}{2n^2}\right)^4 M^2_{nl,E(l+1)}. \tag{14}$$

In the quantum treatment of the motion of the nuclei, the partial wave function of the initial state (normalized at infinity to unity flux density) is given by

$$\Psi_i=\frac{F_{vL}(R)}{R}Y_{LM}(\mathbf{R})\,\Phi_g(\mathbf{r}_1,\mathbf{R})\,\frac{\pi\sqrt{2(2l+3)}}{k}\,\frac{\varphi_{E(l+1)}(r_2)}{r_2}Y_{(l+1),0}(\mathbf{r}_2). \tag{15}$$

The wave function of the final state is

$$\Psi_f=\frac{F_{EL'}(R)}{R}Y_{L'M'}(\mathbf{R})\,\Phi_u(\mathbf{r}_1,\mathbf{R})\,\frac{\varphi_{nl}(r_2)}{r_2}Y_{l0}(\mathbf{r}_2). \tag{16}$$

Here L, M and L', M' are the orbital quantum numbers of the nuclei before and after the collision, and $F_{EL}(R)$ is the energy-normalized radial wave function of the continuous spectrum. It is convenient to quantize the nuclear wave functions also along the direction of motion of the incident electron.

At the chosen normalization of the wave functions of the initial and final states, the cross section of the dissociative recombination takes the form

$$\sigma^{LM,L'M'}_{nl0,E(l+1)0}=2\pi\left|\left\langle\Psi_i\left|\frac{1}{r_{12}}\right|\Psi_f\right\rangle\right|^2. \tag{17}$$

Substituting (15) and (16) in (17), using the dipole-dipole expansion, and integrating over the coordinates of the first electron, we obtain

$$\sigma^{LM,L'M'}_{nl0,E(l+1)0}=\frac{4\pi^3(2l+3)}{k^2}\left(\frac{k^2}{2}+\frac{1}{2n^2}\right)^4$$

$$\times\left|\left\langle\frac{F_v(R)}{R}Y_{LM}(\mathbf{R})\frac{\varphi_{E.(l+1)}(r_2)}{r_2}Y_{(l+1)0}(\mathbf{r}_2)\right.\right.$$

$$\times\left.\left.\left|\frac{d(R)\,(\mathbf{R}\mathbf{r}_2)}{R}\right|\frac{F_{EL'}(R)}{R}Y_{L'M'}(\mathbf{R})\frac{\varphi_{nl}(r_2)}{r_2}Y_{l0}(\mathbf{r}_2)\right\rangle\right|^2. \tag{18}$$

Using the rules for calculating the dipole moments[14] in the integration with respect to the coordinates of the second electron, we obtain

$$\sigma^{LM',L'M'}_{nl0,E(l+1)0}=\frac{4\pi^3(l+1)^2}{k^2(2l+1)}\left(\frac{k^2}{2}+\frac{1}{2n^2}\right)^4 M^2_{nl,E(l+1)}$$

$$\times\left|\left\langle\frac{F_{vL}(R)}{R}Y_{LM}(\mathbf{R})\left|\frac{d(R)\,(\mathbf{R}\mathbf{n})}{R}\right|\frac{F_{EL'}(R)}{R}Y_{L'M'}(\mathbf{R})\right\rangle\right|^2. \tag{19}$$

Here $\mathbf{n}$ is a unit vector in the direction of motion of the incident electron. It is seen from (19) that when l changes by unity L changes by the same amount, while M remains unchanged, i.e., M' must be equal to M. Integrating over the angle variables we obtain

$$\sigma^{LM,(L\pm1)M}_{nl0,E(l+1)0}=\frac{4\pi^3(l+1)^2}{k^2(2l+1)}\left(\frac{k^2}{2}+\frac{1}{2n^2}\right)^4 M^2_{nl,E(l+1)}\frac{(L_{min}+1)^2-M^2}{(2L_{min}+3)\,(2L_{min}+1)}$$

$$\times\left(\int\limits_0^\infty F_{vL}(R)F_{E(L\pm1)}(R)\,d(R)\,dR\right)^2,\quad L_{min}=\min(L, L\pm1). \tag{20}$$

Averaging over M (which is equivalent in the classical case to averaging over the direction of the axis joining the nuclei), we get

$$\sigma^{L,L\pm1}_{nl0,E(l+1)0}=\frac{4\pi^3(l+1)^2}{k^2(2l+1)}\left(\frac{k^2}{2}+\frac{1}{2n^2}\right)^4$$

$$\times M^2_{nl,E(l+1)}\frac{L_{min}+1}{3(2L+1)}\left(\int\limits_0^\infty F_{vL}(R)F_{E(L\pm1)}(R)\,d(R)\,dR\right)^2. \tag{21}$$

The radial integral in (21) has at $L'=L\pm1$ (see below) practically the same value. Summing (21) over $L'=L\pm1$, we obtain

$$\sigma_{nl0,E(l+1)0}=\frac{4\pi^3(l+1)^2}{3k^2(2l+1)}\left(\frac{k^2}{2}+\frac{1}{2n^2}\right)^4 M^2_{nl,E(l+1)}\left(\int_0^\infty F_v(R)F_E(R)d(R)dR\right)^2. \tag{22}$$

In the quasiclassical approximation, the radial wave functions are given by

$$F_v(R)=A(R)\cos\left(\int^R P_i(x)dx\right),$$
$$F_E(R)=\left(\frac{2\mu}{\pi P_f(R)}\right)^{1/2}\cos\left(\int^R P_f(x)dx\right). \tag{23}$$

Here $P_{i,f}$ are the radial momenta of the nuclei. This yields

$$\int_0^\infty F_v(R)F_E(R)d(R)dR\approx\left(\frac{\mu}{2\pi}\right)^{1/2}\int_0^\infty\frac{A(R)d(R)}{[P_f(R)]^{1/2}}\cos\left(\int^R(P_i(x)-P_f(x))dx\right)dR.$$

The integrand oscillates rapidly, and the value of the integral is determined[10] by the coordinate region where $P_i=P_f$ (i.e., by the condition (4)). Confining ourselves to the first term of the expansion of the momentum difference at the point R_E

$$\int^R(P_i(x)-P_f(x))dx=\frac{du_{if}(R_E)}{dR}\frac{\mu}{2P(R_E)}(R-R_E)^2+B(R_E)$$

and taking the smoothly varying functions $A(R), a(R)$, and $P_f(R)$ outside the integral sign, we obtain

$$\int_0^\infty F_v(R)F_E(R)d(R)dR\approx\frac{A(R_E)d(R_E)}{(|du_{ij}(R_E)/dR|)^{1/2}}\cos\left(B(R_E)+\frac{\pi}{4}\right). \tag{24}$$

The constant $B(R_E)$ varies rapidly with changing E. Replacing the square of the cosine in (24) by the mean value $\frac{1}{2}$, we obtain

$$\sigma_{nl0,E(l+1)0}=\frac{4\pi^3d^2(R_E)(l+1)^2}{3k^2|du_{if}(R_E)/dR|(2l+1)}\left(\frac{k^2}{2}+\frac{1}{2n^2}\right)^4 M^2_{nl,El+1}\frac{A^2(R_E)}{2}. \tag{25}$$

This formula is obtained from (14) if the square of the radial wave function $F_v^2(R_E)$ is averaged over the oscillations. In fact, according to (23) we have

$$\langle F_v^2(R_E)\rangle={}^1/_2A^2(R_E).$$

[1] J. N. Bardsley and M. A. Biondi, Adv. Atom. Mol. Phys. **6**, 1 (1970).

[2] B. M. Smirnov, Iony i vozbuzhdennye atomy v plazme (Ions and Excited Atoms in a Plasma), Atmoizdat, 1974.

[3] B. Peart and K. T. Dolder, J. Phys. B **6**, 359 (1973).

[4] R. A. Phaneuf, D. H. Crandall, and G. H. Dunn, Phys. Rev. A **11**, 528 (1975).

[5] M. Vogler and G. H. Dunn, Phys. Rev. A **11**, 1983 (1975).

[6] E. Bauer and T. Y. Wu, Can. Phys. J. **34**, 1436 (1956).

[7] R. L. Wilkins, J. Chem. Phys. **44**, 1884 (1966).

[8] G. V. Dubrovskiĭ and V. D. Ob"edkov, Astron. Zh. **44**, 387 (1967) [Sov. Astron. **11**, 305 (1967)].

[9] S. E. Nielsen and J. S. Dahler, J. Chem. Phys. **45**, 4060 (1966); R. S. Berry and S. E. Nielsen, Phys. Rev. A **1**, 383, 395 (1970); A **4**, 865 (1971).

[10] L. D. Landau and E. M. Lifshitz, Kvantovaya mekhanika (Quantum Mechanics), Fizmatgiz, 1963 [Pergamon, 1968].

[11] D. R. Bates and R. H. G. Reil, Adv. Atom. Mol. Phys. **4**, 13 (1968).

[12] D. R. Bates, J. Chem. Phys., **19**, 1122, 1951.

[13] H. Van Regemorter, Monthly Not. Roy Astron. Soc. **121**, 213 (1960); see: Atomic and Molecular Processes, D. R. Bates, ed., Academic 1962, Russ. transl. Mir, 1964, p. 361.

[14] I. I. Sobel'man, Vvedenie v teoriyu atomnykh spektrov (Introduction to the Theory of Atomic Spectra), Fizmatgiz, 1963, pp. 99, 439.

[15] B. I. Volkov, D. P. Grechukhin, and E. I. Karpushkina, Tablitsy secheniĭ fotoionizatsii atoma vodoroda (Tables of Hydrogen Atom Photoionization Cross Sections), Preprint Moscow Univ., 1965.

[16] I. V. Komarov, P. A. Pogorelyi, and A. S. Tibilov, Opt. Spektrosk. **27**, 198 (1969).

[17] F. Busch and G. H. Dunn, Phys. Rev. A **5**, 1726 (1972).

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