Role of exchange in the excitation of ions by electrons

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It is shown that in a number of cases allowance for exchange may significantly affect the excitation cross sections for allowed transitions at atoms and in ions near the threshold. This is associated with an appreciable cancellation of the direct and the interference terms in the formula for the cross section. From numerical calculations it follows that the rate of excitation of the resonance and of other singlet levels of heliumlike ions in a plasma taking exchange into account turns out to be only half as big as the one without exchange. On the other hand, in the great majority of calculations on the diagnostics of laboratory and astrophysical plasmas it is just the cross sections without exchange that have been utilized until now. Some applications to plasma diagnostics are discussed.

I. INTRODUCTION

Effective cross sections for the excitation of atoms and ions by electrons have wide application in problems of diagnostics of laboratory and astrophysical plasmas. However, until now reliable methods have not been developed for the calculation of cross section for "slow" electrons, i.e., for $E \sim \Delta E$ (ΔE is the excitation energy). For applications usually the Born or the Born-Coulomb (in the case of ions) cross sections are utilized. These approximations yield sensible results even near the threshold, although, strictly speaking, they are inapplicable in this region. However, there is a basis for the expectation that as the charge of the ion increases the accuracy of the Born-Coulomb approximation increases.

For transitions not involving a change of spin the cross sections are usually calculated without taking exchange into account. Numerical calculations show that at least for hydrogen and for hydrogenlike ions the role of exchange is not great (less than 20%). Perhaps it is because of this that the predominant majority of calculations of level populations and intensities is based on cross sections without exchange. And yet numerical calculations and certain model considerations show that for helium and for more complex atoms and ions taking exchange into account can alter the cross section at the threshold by a factor of two or three. It is essential to note that this effect depends very little on the charge of the ion.

In this paper we have investigated the effect of exchange on transitions not involving a change of spin in ions and some examples from plasma diagnostics. It should be emphasized that no new method of calculation is here proposed. The whole consideration is carried out within the framework of the well-known method of Ochkur[1] and of orthogonalized functions[2]. It turns out that the results obtained here can be verified experimentally with the aid of astrophysical data. In subsequent discussion we have used atomic units, with πa_0^2 taken as the unit for the cross section; [A] denotes an ion z from the isoelectronic sequence for the atom A; z is the spectroscopic symbol for the ion.

II. GENERAL DISCUSSION

Since the applicability of the methods of calculation mentioned above[1,2] does not have a rigorous basis near the threshold it appears to be useful to complement the calculations by the following qualitative considerations. From the classical point of view direct excitation corresponds to a transfer of energy ΔE from an external electron to an optical electron, while excitation involving exchange corresponds to a transfer of energy $E^{+}|E_0| - \Delta E \approx E_0$ near the threshold. Here E_0 is the energy of the bound electron in the initial state. For transitions of the type of excitation of [He] from the ground state we have $\Delta E \approx E_0$, and the exchange process practically does not differ from the direct one. Since in this case a considerable amount of energy is transferred, the interaction between the electrons is strong and the binding of the optical electron to the atomic core is severed in the collision process. It is natural to expect that the distribution of products according to spins will be approximately proportional to the statistical weight of the final level $2S_1 + 1$. In the case of transitions between levels lying closely together (for example, $2s - 2p$ in [Be]) $\Delta E \ll E_0$, and the exchange cross section requiring a transfer of a large amount of energy is much smaller than the direct one. The same is true for any arbitrary transition for $E \gg \Delta E$.

We now go over to quantitative methods. As is well known, the Born-Oppenheimer method turns out to be quite useless near the threshold. Two modifications of this method have been proposed[1,2]. In the Ochkur approximation[1] the cross section for the transition $(L_pS_p)n_0l_0L_0S_0 \rightarrow (L_pS_p)n_1l_1L_1S_1$ is equal to

$$\sigma = \frac{8}{k^2}\sum_{\varkappa}\int_{k_0-k_1}^{k_0+k_1}\frac{dq}{q^3}|f_\varkappa|^2\left[\delta_{S_0S_1}\left(1-\frac{q^2}{k_0^2}\right)+\frac{2S_1+1}{2(2S_p+1)}\frac{q^4}{k_0^4}\right]. \qquad (1)$$

Here f_K is the Born amplitude which does not depend on the spins. At the threshold $k_1 = 0$, $q = k_0$ and $\sigma \sim 2S_1 + 1$. Evidently this is connected with the total cancellation of the direct and the interference terms in (1). Thus, in the Ochkur approximation the cross section at the threshold is of order $2S_1 + 1$ independently of the relationship between ΔE and $|E_0|$.

The Ochkur approximation is directly applicable to only to neutral atoms. The method of orthogonalized functions[2] can be utilized both for atoms and for ions. The numerical calculations described below have been carried out by this method. The expression for the cross section is more complicated (cf., Appendix) and includes the factor

$$\delta_{S_0S_1}(f^2-fg)+(2S_1+1)g^2/2(2S_p+1), \qquad (2)$$

where f and g are the direct and the exchange integrals. The degree of proportionality of the result to the statistical weight $2S_1 + 1$ is evidently determined by the degree of cancellation of the direct and the interference terms.

Numerical calculations show that in agreement with the qualitative considerations given above:

1) for $\Delta E \ll |E_0|$ $f \gg g$ and exchange is not significant;

2) for $\Delta E \sim |E_0|$ near the threshold $|f - g| \ll f$, i.e., considerable cancellation occurs; taking exchange into account can be very significant.

In particular, for [He] the quantity $(2S_1 + 1)/2(2S_p + 1) = 1/4$ and the cross sections for the excitation of singlet levels from the ground state $1\,^1S$ turn out to be smaller by a factor of two or three at the threshold than when exchange is neglected. With increasing energy E of the incident electron g/f decreases as $1/E$.

As an illustration Fig. 1 gives cross sections for the excitation of $2\,^1P$- and $2\,^3P$-levels of the ion O VII [He], and Fig. 2 gives cross sections for the transitions $2\,^1S - 2\,^1P$, $2\,^3P$ in O V [Be].

It is important to note that in accordance with (2) the total cross section with respect to S_1 is given by the quantity

$$f^2 - fg + g^2, \qquad (3)$$

which for $|g| \leq |f|$ depends only weakly on exchange. Therefore the numerical results obtained without taking exchange into account should be interpreted as a total cross section with respect to S_1 (cf., Fig. 1).

The relation $|g| \leq |f|$ is not satisfied for quadrupole transitions. Terms of lower multipolarity occur in the exchange amplitude and this leads to a considerable increase in g. Figure 3 shows cross sections for the transitions $1\,^1S - 3\,^1D$, $3\,^3D$ in O VII. As can be seen, at the threshold the cross section for the excitation of the triplet level $\sigma(^3D)$ is considerably greater than $\sigma(^1D)$. It is of interest that even in this case taking exchange into account leads to a decrease in $\sigma(^1D)$. For neutral atoms $\sigma(^1D)$ can be significantly increased as a result of transitions through an intermediate level (in second order)[3]. However, for ions with $z > 4$ this effect is not significant.

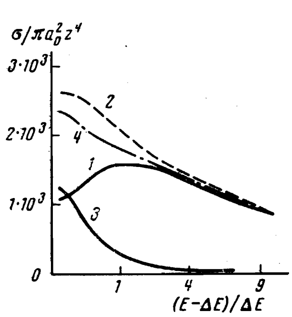

FIG. 1

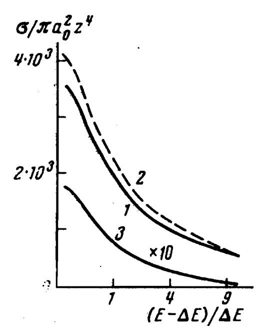

FIG. 2

FIG. 1. Cross sections for the excitation of the 1s-2p transition in the OVII ion: 1- for 2^1P level taking exchange into account, 2- the same without taking exchange into account, 3- for the 2^3P level, 4- the sum of cross sections 1 and 3.

FIG. 2. Cross sections for the excitation of the 2s-2p transition in the OV ion: 1- for the 2^1P level taking exchange into account, 2- without taking exchange into account, 3- for the 2^3P level.

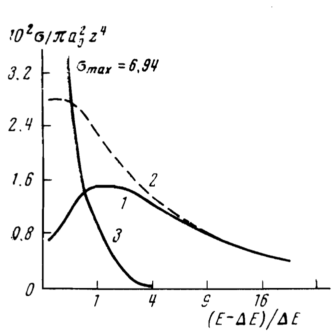

FIG. 3. Cross sections for the excitation of the 1s-3d transition in the OVII ion: 1- for the 3^1D level taking exchange into account, 2- the same without taking exchange into account, 3- for the 3^3D level.

III. EXAMPLES

1. We now consider some applications. Just as in the foregoing, we shall not deal with neutral atoms. For ions the experimental data refer primarily to plasma. Therefore the rates of transitions $\langle v\sigma \rangle$ in the case of a Maxwellian distribution of electron velocities are of particular interest. We make use of the following analytic representation[4]: the transition

$$n_0 l_0^N L_0 S_0 \to n_0 l_0^{N-1} (L_p S_p) n_1 l_1 L_1 S_1, \qquad (4a)$$

the rate of transition

$$\langle v\sigma \rangle = 10^{-8}\,\frac{\text{cm}^3}{\text{sec}} \cdot \left(\frac{E_1 \cdot 1\,\text{Ry}}{E_0 \Delta E}\right)^{3/2} e^{-\beta} b \beta^{1/2} \frac{\beta + \delta_{S_0 S_1}}{\beta + \chi}, \qquad (4b)$$

where

$$\beta = \Delta E/kT, \quad \Delta E = E_1 - E_0, \quad \text{Ry} = 13.6\ \text{eV}$$

The parameters b, χ of the approximation (4b) are chosen by the method of least squares from the results of a numerical calculation of σ and $\langle v\sigma \rangle$. The table gives the values of σ_0 (at the threshold), b and χ for a number of transitions.

2. The cleanest experimental data on the excitation of ions can be obtained from astrophysics. In the x-ray spectrum of the solar corona lines are observed for transitions from the levels 2^1P, 2^3P, 2^3S to the ground state $1\,^1S$ of the [He] ions. In view of low density secondary processes are absent and the ratio of the intensities is given by

$$G \equiv \frac{I(^3P) + I(^3S)}{I(^1P)} \approx \frac{\langle v\sigma(^3P) \rangle + \langle v\sigma(^3S) \rangle}{\langle v\sigma(^1P) \rangle}. \qquad (5)$$

The relation (5) can be violated by only an insignificant amount as a result of population by recombination and cascades.

Cross section at the threshold $^*\sigma_0$ and the parameters b, χ for transitions from the ground state to the final states ^1L, ^3L, ^2L

Transition	^1L			^3L			^2L		
	σ_0	b	χ	σ_0	b	χ	σ_0	b	χ
O VII ion (ground state $1s^2\,^1S$)									
$1s - 2s$	44	6.0	0.52	18.6	2.4	0.37			
$3s$	7.0	4.6	0.40	4.2	2.6	0.42			
$2p$	108	20	0.03	124	16.2	0.68			
$3p$	17.0	15.4	0.02	28	17.0	0.75			
$3d$	0.7	0.78	0.01	7.0	4.0	1.1			
$4d$	0.32	0.96	0.01	3.2	5.2	1.2			
$4f$	0.24	0.44	4.3	—	—	—			
Li II ion (ground state $1s^2\,^1S$)									
$1s - 2s$	38	9.4	0.99	0.66	0.36	−0.14			
$2p$	46	16.8	0.01	26	10.6	0.38			
O V ion (ground state $2s^2\,^1S$) ^1S)									
$2s - 2p$	$3.6 \cdot 10^5$	11.2	0.63	17 600	0.58	0.096			
$3p$	$3.8 \cdot 10^2$	1.9	−0.077	460	1.56	0.39			
$3s$	$2.4 \cdot 10^3$	6.6	0.62	320	0.82	0.45			
O VIII ion (ground state $1s\,^2S$)									
$1s - 2s$	—	—	—	—	—	—	45	4.2	7.5
$2p$	—	—	—	—	—	—	190	17	0.23

*Here σ_0 is in units of $\pi a_0^2/100\,z^4$ where z is the spectroscopic symbol of the ion.

The measured value of G for O VII, Ne IX, Mg XI is close to unity (cf., for example, [5,6]). At the same time the value calculated without taking exchange into account is for singlet transitions G = 0.4. Utilizing the data of the table we obtain G = 0.7–1.0 in the range $\beta = 3-6$ within which the indicated lines are luminous. In fact usually $\beta = 5-6$, and this corresponds to G = 0.9–1, in excellent agreement with the observed value.

3. For resonance lines of the ions of [He] calculations without taking exchange into account yield b = 40[4] which is twice as great as the value given in the table. The same result is given by the frequently used empirical formula due to Van Regemorter [7]. Thus, the theoretical intensities of the [He] lines are in practically all calculations overestimated by a factor of two.

For a determination of the temperature of a hot plasma—both of a laboratory and of an astrophysical plasma—frequently the ratio of intensities of the resonance lines of [He] and [H] is utilized. Figure 4 shows the dependence of this ratio on $\beta_i^{-1} = kT/E_i$ (E_i is the ionization energy for the [He] ion) for the ions of oxygen and of sulphur. It is assumed that the ionization equilibrium is determined by radiative and dielectronic recombination. It can be seen that for not too "low" temperatures (when the intensity of the [H] line is comparable with I [He]) the use of cross sections without exchange taken into account leads to an appreciable error in the temperature.

4. In recent years another method of determining the temperature has become widely used—in terms of the relative intensities of "satellites" near the resonance lines of [He] or of [H] [8,9]. These satellites are due to transitions from the autoionization levels. For example, the transitions $1s2pnl - 1s^2nl$ give rise to satellites of the resonance line of [He] $1s2p\,^1P - 1s^2\,^1S$. In the most important case of dielectron population the relative intensity of the satellite γ is equal to

$$i(\gamma)=\frac{I_s(\gamma)}{I_{res}}=\frac{N_{z-1}(\gamma)A(\gamma-\gamma_0)}{N_zN_e\langle v\sigma_{res}\rangle}, \qquad (6)$$

where $A(\gamma - \gamma_0)$ is the probability of a radiative transition for the satellite.

The population $N_{Z-1}(\gamma)$ of a level "immersed in the continuous spectrum" differs from the population according to Saha by the factor $\Gamma/(\Gamma + A)$ where Γ is the probability of autoionization. Utilizing (5) and setting $\beta \approx 3$ we obtain (g is the statistical weight):

$$i(\gamma)=\frac{1.5\cdot 10^{-15}}{g_0b}\frac{g_\gamma\Gamma(\gamma)A(\gamma-\gamma_0)}{A(\gamma)+\Gamma(\gamma)}n^2\delta\beta e^{\delta\beta}, \quad \delta\beta=\frac{E_i}{n^2kT}. \qquad (7)$$

For the satellites of [H] and [He], according to the table, g_0b is respectively equal to 34 and 20. Without taking exchange into account $g_0b = 40$ in both cases.

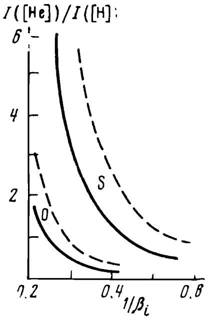

FIG. 4. Dependence of the temperature ($1/\beta_i = kT/E_i$) of the ratio of intensities of the resonance lines of [He] and [H[ions for O and S ions: solid curves—taking exchange into account, dotted curves—without taking exchange into account.

Formula (7) is particularly convenient for determining temperature since satellites are excited from the same initial level as the resonance line. This is important in the case of an inhomogeneous or a rapidly varying plasma. At the same time the correct value of the cross section (of the factor b) is important here since $\delta\beta$ is considerably smaller than β (usually $\delta\beta$ is of the order of magnitude of unity).

5. The ionization equilibrium in a plasma is in many cases determined by dielectron recombination. In this case an additional population of excited levels occurs. We consider the simplest case

$$[\mathrm{H}(1s)]+e\to[\mathrm{He}(2pnlLS)]\to[\mathrm{He}(1snlL'S)]+\hbar\omega. \qquad (8)$$

Distribution over the spin states of the final ion $[\mathrm{He}(1\,snlL'S)]$ is given by the expression

$$\tfrac{1}{4}(2S+1)(f+(-1)^Sg)^2,\quad S=0,\ 1, \qquad (9)$$

with the amplitudes f and g taken at the threshold. Without taking exchange into account (g = 0) the products are distributed in proportion to the statistical weight 2S + 1, i.e., triplets are populated three times more intensely than singlets. However, in actual fact $g \approx f$, and the triplets are practically not populated at all. At the same time the total rate of dielectron recombination is of the order of $f^2 - fg + g^2$ and does not depend strongly on exchange.

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APPENDIX

The cross section (in units of πa_0^2) for the excitation of the transition $0 \to 1$ is given by the expression

$$\sigma([L_pS_p]n_0l_0L_0S_0-[L_pS_p]n_1l_1L_1S_1)=\sum_{\lambda_0\lambda_1\varkappa'\varkappa''}\sigma_{\varkappa'\varkappa''}(\lambda_0\lambda_1), \qquad (A.1)$$

$$\sigma_{\varkappa'\varkappa''}(\lambda_0\lambda_1)=\frac{4\pi^2k_1}{k_0^3}\sum_{L_T}\Big[(A_{\varkappa'}'R_{\varkappa'}')^2-A_{\varkappa'}'A_{\varkappa''}''R_{\varkappa'}'R_{\varkappa''}'' + \frac{2S_1+1}{2(2S_p+1)}A_{\varkappa''}''R_{\varkappa''}''\sum_{\varkappa'''}A_{\varkappa'''}''R_{\varkappa'''}''\Big], \qquad (A.2)$$

where R′ and R″ are the direct and the exchange radial integrals:

$$R_\varkappa'=\int_0^\infty\int_0^\infty P_0(r_1)F_{\lambda_0}(r_2)\left(\frac{r_<^\varkappa}{r_>^{\varkappa+1}}-\frac{\delta_{\varkappa0}}{r_>}\right)P_1(r_1)F_{\lambda_1}(r_2)\,dr_1\,dr_2, \qquad (A.3)$$

$$R_\varkappa''=\int_0^\infty\int_0^\infty P_0(r_1)g_{\lambda_0}(r_2)\frac{r_<^\varkappa}{r_>^{\varkappa+1}}P_1(r_2)g_{\lambda_1}(r_1)\,dr_1\,dr_2;$$

$$g_{\lambda_0}=F_{\lambda_0}-\langle F_{\lambda_0}|P_1\rangle P_1\delta_{\lambda_0l_1}, \qquad g_{\lambda_1}=F_{\lambda_1}-\langle F_{\lambda_1}|P_0\rangle P_0\delta_{\lambda_1l_0}; \qquad (A.4)$$

P_0, P_1 are the radial functions for the optical electron of an atom (ion), F_λ are the functions for the continuous spectrum of an electron of angular momentum λ in a Coulomb field $-(z-1)/r$, normalized to $\delta(k-k')$. The coefficients A′ and A″ are defined in the following manner:

$$A_\varkappa'=\delta_{S_0S_1}(-1)^{L_0+L_1+L_T}(\varkappa l_0l_1)(\varkappa\lambda_0\lambda_1)(L_T)^{1/2}(L_0)^{1/2}(L_1)^{1/2}\times\begin{Bmatrix}\varkappa & L_0 & L_1\\ L_p & l_1 & l_0\end{Bmatrix}\begin{Bmatrix}\varkappa & L_0 & L_1\\ L_T & \lambda_1 & \lambda_0\end{Bmatrix}, \qquad (A.5)$$

$$A_\varkappa''=(-1)^{\varkappa+l_1+\lambda_1+L_p}(\varkappa l_0\lambda_1)(\varkappa\lambda_0l_1)(L_T)^{1/2}(L_0)^{1/2}(L_1)^{1/2}\times\begin{Bmatrix}\lambda_0 & L_T & L_0\\ l_1 & L_1 & L_p\\ \varkappa & \lambda_1 & l_0\end{Bmatrix}, \qquad (A.6)$$

where the following notation has been used:

$$(j_1j_2j_3)=(j_2)^{1/2}(j_3)^{1/2}\begin{pmatrix} j_1 & j_2 & j_3 \\ 0 & 0 & 0 \end{pmatrix},\quad (j)=2j+1. \tag{A.7}$$

In carrying out actual calculations one can usually restrict oneself to a single minimal value κ', κ'', κ''' (taking (A.5) and (A.6) into account):

$$\begin{aligned} \varkappa' &= \max(|l_0-l_1|,\ |\lambda_0-\lambda_1|), \\ \varkappa''=\varkappa''' &= \max(|\lambda_0-l_1|,\ |\lambda_1-l_0|). \end{aligned} \tag{A.8}$$

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9