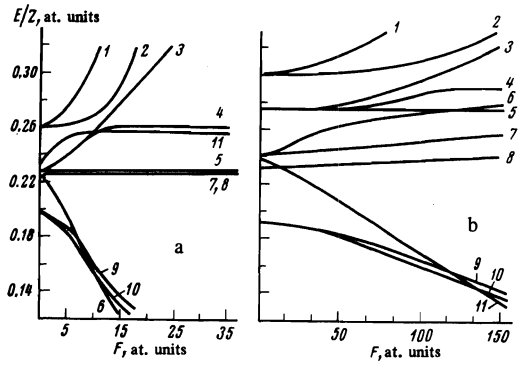


FIG. 2. Dependences of the level energies on the field intensity: a) for $Z=10$; b) for $Z=30$. The numbers alongside the curves are the indices of the levels $E_i$.

ing the addition of momentum and parity conservation. If the levels do not combine, i.e., if the nondiagonal matrix elements of the operator of the external field between the corresponding states vanish, the theorem on the crossing of levels with identical quantum numbers[4] is inapplicable: the levels "do not know" of the existence of one another and there can be no mutual repulsion.

Figure 2 shows dependences of a different kind: the level energies are plotted as a function of the field $F$ for fixed values of $Z$. The maximum values of the field intensity in Fig. 2 are of the order of the internal atomic field for the corresponding values of $Z$. The curves in Fig. 2 demonstrate also repulsion of the levels and the appearance of new crossings in an electric field.

It should be noted that, in contrast to $Z$, the field is a continuous parameter, i.e., we are dealing here with real intersections. In all the graphs the level energies are divided, by convenience, by $Z$ and represented in atomic units; the field intensity $F$ is also given in atomic units (1 at. unit $=5.14\times10^9$ V/cm). It is clear from Figs. 1b and 2 that the influence of an external field of fixed intensity $F$ rises when $Z$ is reduced. This is fairly self-evident: the matrix element of the Coulomb interaction of electrons is proportional to $Z$ and the Stark matrix element is proportional to $Z^{-1}$.

[1]V. G. Gorshkov and L. N. Labzovskiĭ, Pis'ma Zh. Eksp. Teor. Fiz. 19, 768 (1974) [JETP Lett. 19, 394 (1974)].
[2]G. L. Klimchitskaya and L. N. Labzovskiĭ, Opt. Spektrosk. 34, 633 (1973) [Opt. Spectrosc. (USSR) 34, 365 (1973)].
[3]L. N. Labzovskiĭ, Vestn. Leningr. Univ. Ser. Fiz. Khim. No. 2, 19 (1973).
[4]L. D. Landau and E. M. Lifshitz, Kvantovaya mekhanika, Nauka, M., 1974, p. 351 (Quantum Mechanics: Non-Relativistic Theory, 2nd ed., Pergamon Press, Oxford, 1965).

Translated by A. Tybulewicz

# Nonresonant charge exchange in dense gases

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(Submitted July 3, 1975)
Zh. Eksp. Teor. Fiz. **70**, 543–546 (February 1976)

It is shown that the increase of density of a medium can result in a pronounced change in the nonresonant charge exchange cross section, even though the pairing condition for the process is satisfied with sufficient margin. At a large bare resonance defect the final result is determined by competition between an exponentially small cross section corresponding to a nonadiabatic transition and a low probability of particle configurations in the medium such that the effective defect is negligible.

PACS numbers: 82.30.Fi

When the density of a gas medium is increased, its influence on the inelastic collisions of atoms and molecules begins to come into play even before triple collisions become significant. Indeed, this becomes a pairing process if the criterion $n\sigma^{3/2}\ll 1$ is satisfied, where $n$ is the density of the gas and $\sigma$ is the collision cross section.[1)] However, the potential fields produced by the gas environment can lead to a shift of the terms of the colliding particles, which greatly influences the value of $\sigma$ even in the region where the foregoing inequality is satisfied. The corresponding problem was considered earlier[1] with resonant charge exchange as an example, while Lisitsa[2] investigated the crossing of the atomic terms under the influence of a random field of a gas medium. The present paper is devoted to nonresonant charge exchange in gases of finite density, when the criterion for the pairing in the collisions is still satisfied.

According to Massey's adiabatic criterion the cross section for nonresonant charge exchange is exponentially small in comparison with the gas-kinetic cross section if the resonance defect $\Delta$ greatly exceeds the quantity $\gamma v$, where $v$ is the relative collision velocity and $\gamma$ is of the order of the atomic momentum. The ion that takes part in the charge exchange polarizes the particles of the surrounding gas, and this leads to a shift of the terms of the quasi-molecule made up of the colliding atoms. Thus, an effective renormalization of $\Delta$ takes place and, in particular, particle configurations are possible in which the resonance defect is practically completely suppressed, that is, $|\Delta_{eff}|$ becomes less than

or of the order of $\gamma v$. This corresponds to resonant charge exchange, which is characterized by large cross sections. The final result will obviously be determined by the competition between the low probability of the favorable configurations and the exponential smallness of the cross section corresponding to a nonadiabatic transition at a large resonance defect.

The difference between the terms of the quasimolecule in the presence of a gas environment is of the form

$$H_{11}-H_{22}=\Delta-\frac{(\alpha_1-\alpha_2)e^2}{2r^4}+2\alpha e^2\sum_i\frac{\mathbf{rR}_i}{R_i^6}. \tag{1}$$

Here $\Delta$ is the "bare" resonance defect; $\alpha_1$, $\alpha_2$, and $\alpha$ are the polarizabilities of the colliding atoms and particles of the gas medium, respectively; we assume henceforth that the ion exchanges charge with one of the gas atoms, that is, $\alpha=\alpha_2$; $\mathbf{r}$ is the distance between the colliding atoms, $\mathbf{R}_i$ is the coordinate of the $i$-th particle of the gas environment. In formula (1), account is taken of the fact that the distances that are essential for charge exchange are $r\ll R_i$ (pair collisions).[2)]

The charge-exchange probability depends on the effective resonance defects $\Delta_1$ and $\Delta_2$ at the points $r_{c1}$ and $r_{c2}$ (respectively when the atoms come close together or move apart), where the off-diagonal matrix element of the interaction $H_{12}$ becomes comparable with the difference of the diagonal elements $|H_{11}-H_{22}|$. In contrast to collision in vacuum, $\Delta_1$ is in general not equal to $\Delta_2$, so that the points $r_{c1}$ and $r_{c2}$ correspond to different configurations of the quasi-molecule and the gas particles. The binary distribution function of the defects $\Delta_1$ and $\Delta_2$ is of the form[1]

$$f(\Delta_1,\Delta_2)=\frac{1}{4\pi^2}\int_{-\infty}^{+\infty}\int\exp\{i(\Delta_1t_1+\Delta_2t_2)-nA(\alpha e^2)^{3/5}\times[\rho^2(t_1+t_2)^2+x^2(t_1-t_2)^2]^{3/10}\}dt_1\,dt_2, \tag{2}$$

$$A=\frac{5\pi}{3\cdot2^{2/5}}\Gamma\left(\frac{2}{5}\right)\cos\frac{3\pi}{10}\approx5.17,$$

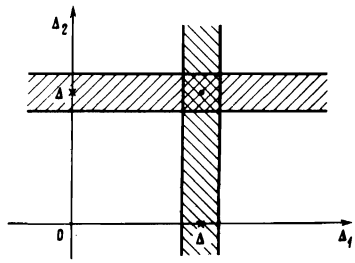
where $\rho$ is the impact parameter of the collision and $x=(r_c^2-\rho^2)^{1/2}$; we assume the atoms to move in straight lines. The quantities $r_{c1}$ and $r_{c2}$ are of respective order of magnitude $\gamma^{-1}\ln(\gamma^2/\Delta_{1,2})$ ($\hbar=1$, $m=1$), and we shall assume with logarithmic accuracy $r_{c1}=r_{c2}=r_c$.

The charge-exchange probability in the case of different defects at two critical points was calculated earlier[1]

$$W=\frac{1}{2}\left[1-\operatorname{th}\frac{\pi|\Delta_1|}{2\gamma v(1-\rho^2/r_{c1}^2)^{1/2}}\operatorname{th}\frac{\pi|\Delta_2|}{2\gamma v(1-\rho^2/r_{c2}^2)^{1/2}}\right]. \tag{3}$$

Formula (3) corresponds to the result averaged over the fast oscillations of the transition probability, which take place at $\rho\lesssim\rho_0\sim\gamma^{-1}\ln(\gamma/v)$. In the region $\rho>\rho_0$, the probability $W$ is practically equal to zero.

The collision cross sections averaged over the configurations are determined by the formula




$$\langle\sigma\rangle=2\pi\int f(\Delta_1,\Delta_2,\rho)W(\Delta_1,\Delta_2,\rho)\rho\,d\rho\,d\Delta_1\,d\Delta_2, \tag{4}$$

and the upper limit in the integration over the impact parameter $\rho_{max}$ depends itself on $\Delta_1$ and $\Delta_2$. Generally speaking, $\rho_{max}=\min(\rho_0,r_{c1},r_{c2})$. We, however, will consider the most interesting case $\Delta\gg\gamma v$, and therefore $\rho_0$ can be excluded from the number of competing values, since $\rho_0>r_{c1}$ and $\rho_0>r_{c2}$ in this case.

As already indicated above, $r_{c1}$ and $r_{c2}$ are equal with logarithmic accuracy, so that $\rho_{max}=r_c$, where $r_c$ is determined by the values of the defects that are important in the integration in (4) with respect to $\Delta_1$ and $\Delta_2$. It is seen from (3) that the probability of the transition differs essentially from zero in that part of the $(\Delta_1,\Delta_2)$ plane which is shown in the figure. The width of the band is of the order of $\gamma v$, and the center of the region is located at the point $\Delta_1=\Delta_2=\Delta$. Thus, $\rho_{max}\approx\gamma^{-1}\times\ln(\gamma^2/\Delta)$.

We present the result of the calculation of the cross section in two limiting cases: at $\Delta\gg\gamma v\gg\alpha e^2r_cn^{5/3}$

$$\langle\sigma\rangle=4r_c^2\frac{\gamma v}{\Delta}\exp\left\{-\frac{\pi\Delta}{\gamma v}\right\}+Br_c^2\frac{n(\alpha e^2r_c)^{3/5}\gamma v}{\Delta^{4/3}}; \tag{5a}$$

at $\Delta\gg\alpha e^2r_cn^{5/3}\gg\gamma v$

$$\langle\sigma\rangle=Br_c^2\frac{n(\alpha e^2r_c)^{3/5}\gamma v}{\Delta^{4/3}}, \tag{5b}$$

where

$$B=\frac{2^{11/5}\ln2}{3}\sqrt{\pi}\,\Gamma\left(\frac{2}{5}\right)\cos\frac{3\pi}{10}\Gamma\left(\frac{8}{10}\right)\Big/\,\Gamma\left(\frac{7}{10}\right)\approx2.01,$$

$$r_c\approx\gamma^{-1}\ln(\gamma^2/\Delta).$$

In formula (5a), the first term corresponds to collision of particles in vacuum,[3] and the second term gives the sought effect of the gas environment.

We present some numerical estimates. At $v\sim10^6$ cm/sec, $\gamma\sim1$ a.u., $\alpha\sim10$ a.u., and $\Delta\sim0.5$ eV the second term of (5a) becomes equal to the first at $n=3\times10^{18}$ cm$^{-3}$; for $n=10^{20}$ cm$^{-3}$ we have $\sigma\sim10^{-2}$ a.u. The condition for the collisions to be binary is still well satisfied in this case: $r_c^3n\sim6\times10^{-4}$.

In the case of charge exchange in a dense strongly ionized plasma, the shifts of the terms of the quasimolecule are determined by the Coulomb field of the charged particles. It can be easily shown that the density-dependent part of the cross section, that is, the second term in (5a) and formula (5b), takes the form (at $\Delta\gg e^2r_cn^{2/3}$)

$$\langle\sigma\rangle=\frac{16\pi\ln 2}{15}r_c^2\frac{n_i(e^2r_c)^{1/4}\gamma v}{\Delta^{3/2}}\approx 2.35r_c^2\frac{n_i(e^2r_c)^{1/2}\gamma v}{\Delta^{3/2}},\qquad(6)$$

where $n_i$ is the ion density. At the parameter values used above, the coefficient of $n_i$ in (6) is approximately two orders of magnitude larger than the coefficient of $n$ in (5). A characteristic feature of the obtained formulas is the linear increase of the cross section with increasing velocity.

The foregoing calculations are based on the assumption that the quantum-mechanical part of the problem, that is, the calculation of the charge-exchange probability, can be solved in the two-particle approximation. This means that the effective charge-exchange radius $r_c$ is small in comparison with the significant distances $R_i$ to the particles of the gas environment. In both considered cases (neutral gas and strongly ionized plasma) the resonance defect is assumed to be large in comparison with the characteristic dimension of the function $f(\Delta_1, \Delta_2)$. Therefore the significant $R_i$ can be estimated from the relations

$$|\Delta-(\alpha_i-\alpha)e^2/2r_c^4|\sim 2\alpha e^2r_c/R_i^5,\quad \Delta\sim e^2r_c/R_i^2$$

for the polarization and Coulomb interactions, respectively. This leads to the following restrictions on $\Delta$:

$$|\Delta-(\alpha_i-\alpha)e^2/2r_c^4|\ll 2\alpha e^2/r_c^4,\qquad(7a)$$

$$\Delta\ll e^2/r_c.\qquad(7b)$$

The compatibility of the inequalities (7a) and (7b) with the conditions for the applicability of formulas (5a), (5b), and (6) is ensured by the criterion $nr_c^3\ll 1$ under which the collisions are binary. Numerical estimates, on the other hand, show that the condition (7b), which pertains to the Coulomb case, can be easily satisfied for many pairs of colliding atoms, whereas (7a) imposes more stringent limitations on the parameters of the collision partners. An example is charge exchange of the nitrogen ion in krypton

$$\Delta=0.54\,\text{eV},\quad \alpha_{Kr}=16.8\ \text{a.u.},\quad \alpha_N=8\ \text{a.u.},\quad r_c=4\ \text{a.u.},$$
$$|\Delta-(\alpha_{Kr}-\alpha_N)e^2/2r_c^4|\approx 2\cdot 10^{-3}\ \text{a.u.},\quad 2\alpha_{Kr}e^2/r_c^4\approx 0.13\ \text{a.u.}$$

In many cases both sides of inequality (7a) are of the same order of magnitude, so that we are at the limit of the region of applicability of formulas (5). It is easily understood, however, that in this case the linear dependence of $\langle\sigma\rangle$ on the product $nv$ is preserved here: the factor $\gamma v$ results from integration of the transition probability $W$, and the proportionality of the density is connected with the fact that $\langle\sigma\rangle$ contains the asymptotic form of the distribution function at large values of $\Delta_1$ or $\Delta_2$. This asymptotic form is determined by the probability that the nearest neighbor will fall in a specified layer, and this in fact governs the value of $n$.

In the case $\Delta\gg e^2/r_c^4$ we cannot use the expansion in the ratio $r_c/R_i$. Then the particles of the gas environment have practically no effect on the cross section of the process if the charge exchange is with one of them. However, the influence of the gas environment may turn out to be appreciable if the given pair is charge-exchanged in a buffer gas whose particles cannot take part in the charge exchange (for example the reaction $A^-+B\to A+B^-$ in an environment of inert-gas atoms which do not form negative ions). Then the transition probability is determined as before by the two-particle formula (3). The condition $\Delta\gg\alpha e^2/r_c^4$ denotes that to suppress the defect the buffer-gas atom must come closer to one of the collison partners than the distance $r_c$, that is, it suffices to take into account the interaction with just this particle. Then the density-dependent part of the cross section takes the form

$$\langle\sigma\rangle=\frac{2^{1/4}\pi\ln 2\cdot n(\alpha e^2)^{1/4}\gamma v}{3\Delta^{7/4}}r_c^2.\qquad(8)$$

We note in conclusion one more situation wherein a sufficiently dense gas environment can qualitatively change the picture of a paired inelastic process. If the reaction proceeds with absorption of energy and the resonance defect exceeds the kinetic energy of the colliding particles, then for collisions in vacuum this process is forbidden by the energy conservation law. The interaction with the atoms of the medium can change the magnitude and even the sign of the resonance defect, and consequently make such a process allowed. This problem, however, encounters a difficulty of its own because it is not clear whether it can be treated by the parametric method, since the trajectory of the atoms is itself determined by transitions in the electron subsystem.

[1)]It is understood that the probability of the transition in the significant region of the impact parameters is of the order of unity.

[2)]The limits of applicability of the result are discussed below.


[1]R. Z. Vitlina and A. M. Dykhne, Zh. Eksp. Teor. Fiz. 64, 510 (1973) [Sov. Phys.-JETP 37, 260 (1973)].

[2]V. S. Lisitsa, Zh. Eksp. Teor. Fiz. 65, 879 (1973) [Sov. Phys.-JETP 38, 435 (1973)].

[3]B. M. Smirnov, Atomnye stolknoveniya i élementarnye protsessy v plazme (Atomic Collisions and Elementary Processes in a Plasma), Atomizdat, 1968.



Translated by J. G. Adashko