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THE CLASSICAL THEORY OF RESONANCE CHARGE EXCHANGE

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The cross section for the resonance charge exchange of an ion on an excited atom is calculated for the case when the charge exchange is determined by the barrierless transition of an electron from the field of one ion into the field of another one. An estimate is made of the range of applicability of the classical theory.

1. The resonance charge exchange of an ion on an atom associated with the transition of a valence electron from one atomic core to another one plays an important role in different phenomena which occur in a plasma. For atoms existing in the ground state the resonance charge exchange at not very high energies of collision is associated with the tunnelling transition of an electron from one atomic core to another one. In this case as the ionization potential I of the atom decreases the cross section for the resonance charge exchange increases as 1/I and it is this case that is discussed in detail in the literature. But as the binding energy of the electron decreases the barrierless transition of an electron from one atomic core to another one plays an ever increasing role since in this case the cross section for resonance charge exchange is proportional to $1/I^2$[1,2]. Therefore, in order to obtain the cross section for the resonance charge exchange of an ion on an excited atom it is necessary to utilize the theory of the barrier-less transition of an electron. All the more so since the classical theory enables one to make an estimate of the cross section for resonance charge exchange for atoms of an alkali metal which are in the ground state[3].

A calculation of the cross section for the resonance charge exchange on an excited hydrogen-like atom was carried out by Bates and collaborators both in the quantum mechanical case[4] and also in the classical case[5,6]. In both these cases it was assumed that in the process of transition the state of the electron described by the quantum numbers n, n_1, m is not changed. We regard such an approach to be incorrect. Simple estimates made on the basis of perturbation theory show that in such a system quite intense transitions take place between states with nearly the same energy. These transitions are due to the motion of the nuclei. As regards the energy of the electron, it practically is not transferred to the nuclei due to the difference in the masses of the electron and the nuclei.

2. Thus, in calculating the probability of transition of a classical electron from the field of influence of one ion into the field of influence of another one for not very high velocities of the nuclei one can assume that the energy of the electron is not changed in the process of collision. It is equal to $-I$, where I is the ionization potential of the excited atom prior to collision. In this case a barrierless transition of an electron from one ion to another one is possible if the potential for the interaction between electrons and nuclei at the midpoint of the axis joining them exceeds the ionization potential of the atom. From this it follows that the classical transition of an electron from one nucleus to another one is possible when the distance between the nuclei is $R < R_0$, where $R_0 = 4e^2/I$. From this the maximum cross section for classical charge exchange (the probability of transition of an electron is less than or equal to $1/2$) is equal to[1,2]

$$\sigma_0 = {}^1/_2\pi R_0^2 = 8\pi e^4 / I^2. \tag{1}$$

This takes place at very small velocities of collision. For arbitrary velocities of collision from considerations of dimensionality (we have at our disposal the parameters I, e; m is the mass of the electron, v is the relative velocity of collision of the nuclei) we represent the cross section for charge exchange in the form

$$\sigma = \sigma_0 f(z), \quad \sigma_0 = \frac{8\pi e^4}{I^2}, \quad z = \frac{v}{\sqrt{2I/m}}. \tag{2}$$

Here f(0) = 1. Our problem is to evaluate the function f(z) for arbitrary z.

3. We consider charge exchange for a given impact parameter in a nuclear collision. Let w_1 be the probability of finding the electron in the field of the first ion, w_2 be the probability of finding it in the field of another ion, j_{12} be the probability of transition of the electron per unit time from the field of the first ion into the field of the second ion and j_{21} be the frequency of the inverse transition. From considerations of symmetry $j_{12} = j_{21} = j$, so that for the probabilities w_1 and w_2 we have the system of balance equations:

$$\frac{dw_1}{dt} = -\frac{dw_2}{dt} = -jw_1 + jw_2.$$

Solving this equation with the initial conditions $w_1 = 1$ and $w_2 = 0$ for $t = -\infty$, we obtain for $t = +\infty$

$$w_2 = \frac{1-e^{-s}}{2}, \quad s = \int_{-\infty}^{+\infty} 2j\, dt.$$

From this, introducing $x = \rho/R_0$ (ρ is the impact parameter for the collision), we obtain for the cross section for resonance charge exchange

$$\sigma = \frac{\pi R_0^2}{2}\left(1 - \int_0^1 2x\, dx\, e^{-s}\right),$$

i.e.,

$$f(z) = 1 - \int_0^1 2x\, dx \exp\left[-\int_x^1 \frac{4R_0 j}{v} \frac{y\, dy}{\sqrt{y^2 - x^2}}\right]. \tag{3}$$

Here we have utilized the law of free relative motion: $R^2 = \rho^2 + v^2t^2$; we have taken into account the fact that as the barrier appears ($R > R_0$) classical transition ceases ($j = 0$) and we have introduced $y = R/R_0$.

4. In finding the frequency of transition of the electron j from the field of influence of one ion into the field of influence of another one we utilize the laws of statistical mechanics. In this case in accordance with the physical conditions of the process we assume that the transitions between states of the electron with different angular momenta and components of angular momentum occur sufficiently rapidly so that the frequency of transition is determined by the binding energy of the electron I. This frequency of transition is equal to

$$j = \int_S \frac{Nv}{4} dS.$$

Here S is the part of the plane drawn through the midpoint of the axis joining the nuclei and perpendicular to it, where the classical electrons can be found, v is the electron velocity and N is the electron density.

From the law of conservation energy the velocity of the classical electron is equal to

$$v = \sqrt{\frac{2}{m}\left(\frac{e^2}{r_1} + \frac{e^2}{r_2} - I\right)}, \tag{4}$$

where r_1 and r_2 are the distances of the electron from the corresponding nuclei. In this case in accordance with the laws of statistical mechanics the probability of finding an electron with the given total energy I in the neighborhood of a given point is proportional to the number of states of the electron, i.e.,

$$N\,d\mathbf{r} = \int \frac{d\mathbf{p}\,d\mathbf{r}}{(2\pi\hbar)^3} \delta\left(\frac{p^2}{2m} - I + \frac{e^2}{r_1} + \frac{e^2}{r_2}\right) \sim v\,d\mathbf{r}.$$

Normalizing the electron density by the condition that it is concentrated in the field of one of the nuclei we obtain from this for the frequency of transition of the electron:

$$j = \frac{1}{2}\left(\int_\Omega \sqrt{\frac{e^2}{r_1} + \frac{e^2}{r_2} - I\,d\mathbf{r}}\right)^{-1} \int_{r<4e^2/I} \sqrt{\frac{2}{m}\left(\frac{2e^2}{r} - I\right)} 2\pi\rho\,d\rho.$$

Here Ω is the coordinate region where in accordance with the laws of classical mechanics the electron can be found with energy $-I$, ρ is the distance from the axis joining the nuclei, $r = \sqrt{\rho^2 + R^2/4}$. Introducing elliptic coordinates we obtain from this

$$j = \frac{1}{\sqrt{2m}} \frac{(1-y)^2}{R_0^{3/2} I(y)}$$

where

$$y = \frac{R}{R_0} \leqslant 1, \quad I(y) = y^{5/2} \int_0^1 d\eta \int_1 d\xi \sqrt{(\xi^2 - \eta^2)\left[\xi - y(\xi^2 - \eta^2)\right]},$$

$$a = \frac{1}{2y} + \sqrt{\frac{1}{4y^2} + \eta^2}. \tag{5}$$

Values of the function I(y) for a number of values y are given below:

y:	0	0.2	0.4	0.6	0.8	1.0
$I(y)$:	0.196	0.194	0.185	0.165	0.136	0.104

Calculated with the aid of formula (5) and of the data quoted above the values of the function f(z) have the asymptotic form:

$$f(z) = \begin{cases} 0.38z^{-1}, & z \to \infty \\ 1 - 0.8z^{2/5}, & z \to 0. \end{cases} \tag{6}$$

Correspondingly the classical cross section for resonance charge exchange in these limiting cases is equal to

$$\sigma_{\text{cl}} = \begin{cases} 13{,}5 e^4 I^{3/2} m^{-1/2} v^{-1}, & v \gg \sqrt{2I/m} \\ \dfrac{8\pi e^4}{I^2}\left[1 - 0.8\left(\dfrac{v\sqrt{m}}{\sqrt{2I}}\right)^{2/5}\right], & v \ll \sqrt{\dfrac{2I}{m}}. \end{cases} \tag{7}$$

The function f(z) for intermediate values of z can be well approximated by the formula

$$f(z) = [1 + 0.8z^{2/5} + 2.6z]^{-1}.$$

5. We determine the domain of applicability of the classical theory and its connection with the quantum theory of resonance charge exchange. The result obtained above is violated at very high velocities of collision, where the inelastic cross sections of collision with an appreciable change in the binding energy of the electron turn out to be comparable with the charge exchange cross section. At very low velocities of collision the sub-barrier transitions of an electron become important which are not taken into account by the classical theory. Therefore, the domain of applicability of the classical theory of resonance charge exchange is restricted both from the side of high velocities as well as the side of low velocities of collision.

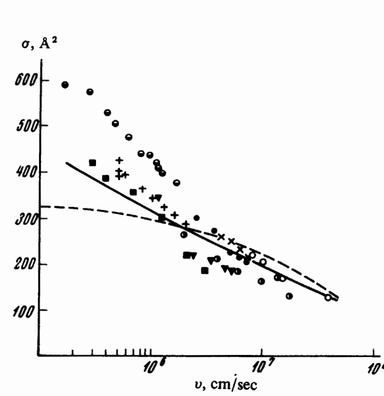
We estimate the domain of applicability of the classical theory from the side of low velocities on the basis of the results of quantum theory for a sub-barrier transition. Thus, if the electron is in an s-state, then the quantum theory of a sub-barrier transition gives for the cross section of resonance charge exchange[7]:

$$\sigma = \frac{\pi R_0^2}{2}, \quad 0{,}28v = \sqrt{\frac{\pi R_0}{2\gamma}} \frac{R_0}{4}\left(\frac{4}{e}\right)^{1/\gamma} \psi^2\left(\frac{R_0}{2}\right).$$

Here $\psi(R_0)$ is the radial wave function for an electron in an isolated atom normalized to unity, $\gamma = \sqrt{2I}$, and the system of atomic units has been utilized. Utilizing the asymptotic expression for the wave function of an s-electron situated in the field of a Coulomb center[8], and introducing the effective principal quantum number $n = 1/\gamma$ we obtain from this

$$\sigma = \frac{\pi R_0^2}{2}, \quad v = \frac{1}{0.28}\sqrt{\frac{\pi}{2}}\left(\frac{4}{e}\right)^n \left(\frac{R_0}{n}\right)^{2n-1/2} e^{-R/n}(n!)^{-2}. \tag{8}$$

We establish the boundary of the classical theory at the point where the cross section for resonance charge exchange obtained by means of formula (8) exceeds the maximum classical cross section of charge exchange (1) ($R_0 \geq 8a_0n^2$, a_0 is the Bohr radius). This gives for



The resonance charge exchange for a Cesium ion on Cesium. Solid line—quantum theory, --- classical theory; experiment: ■–[9], ○–[10], ▽–[11], ●–[12], ◑–[13], ⊗–[14], ◒–[15], +–[16].

the limiting velocity for which the classical theory is applicable expressed in atomic units:

$$v_{\lim} = 0.7 \cdot 0.23^{n} n^{-3/2}. \quad (9)$$

In obtaining this formula we have replaced n! by its asymptotic expression.

For $v > v_{\lim}$ the quantum theory of resonance charge exchange ceases to be applicable since in utilizing it we choose the asymptotic expression for the atomic wave function. As follows from formula (9), the limiting velocity is the smaller, the greater is n, i.e., as could be expected, the applicability of classical theory is the broader the smaller is the ionization potential of the atom I.

The figure shows a comparison between the quantum and the classical theories for the charge exchange of an ion on an atom of Cesium within the domain of applicability of the classical theory. Here are also given results of experiments[9-16].

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[1] L. A. Sena, Zh. Eksp. Teor. Fiz. 9, 1320 (1939).

[2] L. A. Sena, Stolknoveniya elektronov i ionov s atomami (Collisions of Electrons and Ions with Atoms), Gostekhizdat, 1948.

[3] B. M. Palyukh and L. S. Savchin, Zh. Tekh. Fiz. 38, 1055, 1061 (1968) [Sov. Phys.-Tech. Phys. 13, 878 (1969)].

[4] D. R. Bates and R. H. G. Reid, J. Phys. 2B, 851 (1969).

[5] D. R. Bates and R. A. Mapleton, Proc. Phys. Soc. 87, 657 (1966).

[6] D. R. Bates and R. H. G. Reid, J. Phys. 2B, 857 (1969).

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

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

[9] R. M. Kushnir, B. M. Palyukh and L. A. Sena, Izv. Akad. Nauk SSSR, Ser. fiz. 23, 1007 (1959).

[10] D. V. Chkuaseli, V. D. Nikolaishvili and A. I. Guldamishvili, Zh. Tekh. Fiz. 30, 817 (1960) [Sov. Phys.-Tech. Phys. 5, 770 (1961)]; Izv. Akad. Nauk SSSR, Ser. fiz. 24, 970 (1960).

[11] R. M. Kushnir and I. M. Buchma, Izv. Akad. Nauk SSSR, Ser. fiz. 24, 986 (1960).

[12] L. L. Marino, A. C. H. Smith and E. Caplinger, Phys. Rev. 128, 2243 (1962).

[13] J. Perel, R. H. Vernon and H. Daley, Phys. Rev. 138A, 937 (1965).

[14] L. L. Marino, Phys. Rev. 152, 46 (1966).

[15] B. M. Palyukh and L. S. Savchin, Zh. Tekh. Fiz. 38, 1055 (1968) [Sov. Phys.-Tech. Phys. 13, 878 (1969)].

[16] W. R. Gentry, V. Lee and B. H. Mahan, J. Chem. Phys. 49, 1758 (1968).

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140