

RESONANCE CHARGE EXCHANGE IN HYDROGEN AND SODIUM

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Two problems are considered within the framework of the parametric method: 1) Resonance charge exchange of protons in atomic hydrogen. Its probability at all velocities can be expressed through a single integral involving Hankel functions. A numerical calculation is carried out for a single value of the velocity v of the relative motion of the nuclei. 2) Single resonance charge exchange of Na^+ ions in sodium. Up to the present, charge exchange involving complex atoms has been considered in the hydrogen-like approximation. In this article, the calculation is based on analytical wave functions and the analytical expression for the field of the atomic core. These expressions approximate the corresponding quantities computed by the Hartree-Fock method. Results are obtained for all values of v (within the limits of applicability of the parametric method).

1. INTRODUCTION

COLLISIONS between atomic systems for which the energy of the relative motion is of the order 1 eV and higher are most conveniently studied by means of the parametric method.¹⁻⁵

We shall consider the charge exchange

$$(A + e) + B \rightarrow \dot{A} + (B + e), \tag{1}$$

where A and B are certain atomic systems. Its probability is given with sufficient accuracy by the formula*

$$\begin{aligned} \omega_{n_A n_B} = |A_{n_A n_B}|^2 &\equiv \left| \int_{-\infty}^{\infty} \exp\left\{-i\frac{v^2}{2}t + iE_{n_B}t - iE_{n_A}t\right. \right. \\ &+ i \int \langle \psi_{n_B} | V_A | \psi_{n_B} \rangle dt \\ &- i \int \langle \psi_{n_A} | V_B | \psi_{n_A} \rangle dt \left. \right\} dt \int \psi_{n_B}^*(\mathbf{r} - \mathbf{s}) [V_B(|\mathbf{r} - \mathbf{s}|) \\ &- \langle \psi_{n_A} | V_B | \psi_{n_A} \rangle] e^{i\mathbf{v}\mathbf{r}} \psi_{n_A}(\mathbf{r}) d\mathbf{r} \right|^2, \end{aligned} \tag{2}$$

in which ψ_{n_A} (or ψ_{n_B}) and E_{n_A} (or E_{n_B}) are the eigenfunction and energy, respectively, of an electron bound to nucleus A (or B) in the state n_A (or n_B); V_A and V_B are the interaction energies between the electron and nuclei A and B ; \mathbf{s} is the trajectory of the relative motion of the "nuclei." Formula (2) is valid for $\omega_{n_A n_B} \ll 1$. Its derivation can be found, for example, in the paper of Bates.⁵

For (symmetric) resonance, when $E_{n_A} = E_{n_B}$,

$$\langle \psi_{n_A} | V_B | \psi_{n_A} \rangle = \langle \psi_{n_B} | V_A | \psi_{n_B} \rangle$$

(and v^2/Z_A and $v^2/Z_B \ll 1$, where Z_A and Z_B

*Atomic units are used throughout.

are the effective charges of nuclei A and B), formula (2) gives a value of $\omega_{n_A n_B}$ much greater than unity. In this case, we should use, instead of (2),

$$\omega_{n_A n_B} = \sin^2 |A_{n_A n_B}|. \tag{3}$$

In fact, (3) coincides with the formula for the probability of resonance charge exchange obtained by Firsov³ and Demkov⁴ if in the latter the molecular terms are calculated in the first-order approximation of perturbation theory. For $|A_{n_A n_B}|^2 \ll 1$, formula (3) goes over into (2).

2. RESONANCE CHARGE EXCHANGE OF PROTONS IN ATOMIC HYDROGEN

By (2) and (3), the probability of the process is given by the formula

$$\omega = \sin^2 |J_1 - J_2|, \tag{4}$$

where

$$\begin{aligned} J_1 &= \frac{1}{\pi} \int_{-\infty}^{\infty} \exp\left(-i\frac{v^2}{2}t\right) dt \int \frac{1}{|\mathbf{r} - \mathbf{s}|} \exp(-r - |\mathbf{r} - \mathbf{s}| \\ &+ i\mathbf{v}\mathbf{r}) d\mathbf{r}, \\ J_2 &= \frac{1}{\pi} \int_{-\infty}^{\infty} \exp\left(-i\frac{v^2}{2}t\right) [s^{-1} + (s^{-1} + 1)e^{-2s}] dt \int \exp(-r \\ &- |\mathbf{r} - \mathbf{s}| + i\mathbf{v}\mathbf{r}) d\mathbf{r}. \end{aligned}$$

As usual, we neglect the curvature of the trajectory of the relative motion of the nuclei, i.e., we set

$$\mathbf{s} = \boldsymbol{\rho} + \mathbf{v}t, \quad \boldsymbol{\rho}\mathbf{v} = 0 \tag{5}$$

(ρ is the collision parameter). In the case of resonance, this introduces no error.

The integral J_1 has been calculated by Brinkman and Kramers.¹

$$J_1 = \frac{2\rho^2}{v(1+v^2/4)} K_2(\rho\sqrt{1+v^2/4}).$$

We shall now consider the determination of J_2 (see Appendix). The occurrence of this term results from the physical condition that the chosen perturbation be a minimum (in a certain sense), or more precisely, from the fact that the mean value of the perturbation in the state described by the electronic wave function is equal to zero. We find that

$$J_2 = \frac{32}{\pi v} \int_{-\infty}^{\infty} \left[K_0(\rho|\xi|) - K_0(\rho\sqrt{4+\xi^2}) - \frac{2\rho}{\sqrt{4+\xi^2}} K_1(\rho\sqrt{4+\xi^2}) \right] \left\{ \frac{2}{(2v\xi)^2} [K_0(\rho R_+) - K_0(\rho R_-)] + \frac{\rho}{2(2v\xi)^2} \left[\frac{K_1(\rho R_+)}{R_+} + \frac{K_1(\rho R_-)}{R_-} \right] \right\} d\xi, \quad (7)$$

$$R_{\pm} = \sqrt{1+(\xi \pm v/2)^2}.$$

Bassel and Gerjuoy⁶ derived an expression for the probability of the process [where the term (7) was written as a single integral of more complex form]. Along with this, they obtained, by Born's method, an analytical expression for the probability of the process as a function of the scattering angle. Hence the calculations by Born's method in explicit form can be advanced somewhat further. This method, however, is applicable only at large velocities, while the parametric method permits the construction of an approximation that is suitable for small v .

The numerical calculations were performed for an energy 100 kev ($v = 2$). Here $|J_1 - J_2|^2 \ll 1$ for all ρ , and the total cross section was calculated from the formula

$$\sigma = \int_0^{\infty} |J_1 - J_2|^2 2\pi\rho d\rho. \quad (8)$$

Our curve for the probability $|J_1 - J_2|^2$ and the curve given by Bassel and Gerjuoy⁶ turned out to be identical.

For the total cross section, we found the value $\sigma = 0.34$. The following values were found by Bassel and Gerjuoy,⁶ Jackson and Schiff⁷ (in whose paper the term $\langle \psi_{nA} | V_B | \psi_{nA} \rangle$ was replaced by s^{-1}), and Brinkman and Kramers¹ (the perturbation contains only the term V_B): $\sigma_{BG} = 0.32$, $\sigma_{JS} = 0.26$, and $\sigma_{BK} = 1.26$. Hence, for medium v ($v^2 \sim 1$), the results of Jackson and Schiff⁷ are more accurate than those of Brinkman

and Kramers,¹ while for large v ($v^2 \gg 1$), the value σ_{BK} , and not σ_{JS} , coincides with the accurate value.⁶

3. RESONANCE CHARGE EXCHANGE OF SINGLY CHARGED POSITIVE SODIUM IONS IN SODIUM

We shall calculate this process in order to see how accurately the universal formulas obtained in a number of papers* on the basis of the approximation involving hydrogen-like functions describes a single charge exchange.

We assume that the charge exchange involves only the outer 3s electron and we employ the analytical wave functions⁹ and the analytical expression for the field of the atomic core obtained by I. V. Abarenkov (private communication);

$$\psi_{30}(r) = 0.1704(1 - 5.268r + 4.013r^2)e^{-r}r \quad (9)$$

(this function was normalized to 4π);

$$V_B(r) = r^{-1}\{1 + 15.85e^{-3.6r} - 5.85e^{-16.1r} - 75.2re^{-9.9r}\}. \quad (10)$$

Proceeding along the lines indicated in the Appendix, we obtain an expression for the probability amplitude of the process A in terms of a large number of integrals of the form†

$$J_{mn}(\alpha, \beta) = \int_{-\infty}^{\infty} \exp\left(-i\frac{v^2}{2}t\right) dt \int \exp(-\alpha r - \beta|r-s| + i\mathbf{v}\mathbf{r}) r^{m-1} |r-s|^{n-1} dr = (-1)^{m+n} (\partial^{m+n}/\partial\alpha^m \partial\beta^n) J_{00}(\alpha, \beta); \quad (11)$$

$$J_{00}(\alpha, \beta) = \frac{8\pi}{v(\alpha^2 - \beta^2)} \left[K_0\left(\rho\sqrt{\beta^2 + \frac{v^2}{4}}\right) - K_0\left(\rho\sqrt{\alpha^2 + \frac{v^2}{4}}\right) \right]. \quad (12)$$

The extremely cumbersome calculations were carried out by the method suggested by Demkov,⁴ i.e., the cross section was determined from the formula

$$\sigma = \frac{1}{2} \pi \rho_0^2 + \int_{\rho_0}^{\infty} |A|^2 2\pi\rho d\rho, \quad (13)$$

where ρ_0 is the largest root of the equation

$$|A|^2 = 1/2 \quad (14)$$

(in the case of those v for which $|A|^2 < 1/2$, we take $\rho_0 = 0$). The results are shown in the table, in which σ_1 are the results of the present work, σ_2 are those obtained previously,⁸ and σ_e are the

*In the papers of Firsov³ and Demkov,⁴ the corresponding calculations were limited to small v ; the present author obtained results⁸ which were valid for both small and large v .

†We do not include the term $\langle \psi_{nA} | V_B | \psi_{nA} \rangle$ here.

Cross section	v^*			
	0.00026	0.0037	6	$v \rightarrow \infty$
σ_1	385	270	0,00167	$3.8 \cdot 10^4 v^{-12}$
σ_2	388	272	0,00915	$1.3 \cdot 10^3 v^{-12}$
σ_e	329	164	—	—

experimental data.¹⁰ The table also gives expressions for $\sigma(v)$ as $v \rightarrow \infty$.

For the lowest value of the velocity ($v^2 = 0.00026$), the cross section was also calculated by Firsov's method.³ The value obtained here is somewhat greater (by less than 10%) than that shown in the table.

It is seen from the table that for small v (in the case of resonance charge exchange), the hydrogen-like approximation is accurate. In view of the fact that, for small v , the cross section has the form⁴

$$\sigma(v) = (a - b \ln v^2)^2, \quad (15)$$

its value at two points completely determines the shape of the curve.

For large v , the calculations with hydrogen-like functions lead to results that are correct only as regards the order of magnitude. This is explained by the fact that there is such a sizable decrease in the effective distance of charge exchange that the detailed behavior of the wave function and the perturbation energy close to the origin prove to be important. The size of the cross section is then determined by two competitive factors: 1) At small distances between the electron and the incident nucleus, the effective charge is much larger than in the hydrogen-like approximation. 2) The probability of the electron being close to the nucleus is much less than in the hydrogen-like approximation.

It should be noted that, at very large v , inelastic transitions of 2p and 2s, and then 1s electrons begin to play the main role as the energy increases.* If we estimate the charge-exchange cross section for $v^2 \gg 400$ (energy much greater than 200 Mev), when captures of 1s electrons are most important, then it turns out that it is of the same order of magnitude as in the case of the capture of an electron bound to a "bare" sodium nucleus by another such nucleus (i.e., the result obtained by Brinkman and Kramers¹ is 2×10^7 times that shown in the fourth column of the table ($v \rightarrow \infty$)).

Thus, for v^2 in the range

*Since the second factor indicated above is not involved in these transitions.

$$6 < v^2 < 400 \quad (16)$$

the charge-exchange cross section drops much more slowly than v^{-12} , and only for v^2 of the order 1000 does it begin to fall off like v^{-12} . If it is necessary to make a rough estimate of the cross section in the range (16), its value for $v^2 = 6$ (third column of the table) should be matched to the value for v^2 of the order 1000.

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APPENDIX

Using the Fourier transformation

$$r^{-1} e^{-\gamma r} = \frac{1}{2\pi^2} \int \frac{\exp(ikr) dk}{\gamma^2 + k^2},$$

we rewrite the expression for J_2 in the form

$$J_2 = \frac{8}{\pi^2 v} \int_{-\infty}^{\infty} \left[\frac{1}{\sqrt{x^2 + \rho^2}} - \left(1 + \frac{1}{\sqrt{x^2 + \rho^2}} \right) \exp(-2\sqrt{x^2 + \rho^2}) \right] \times dx \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{\exp(ix\xi + i\rho\eta) d\xi d\eta d\zeta}{[1 + (\xi + v/2)^2 + \eta^2 + \zeta^2]^2 [1 + (\xi - v/2)^2 + \eta^2 + \zeta^2]^2}.$$

Integrating over x , we obtain (see ref. 11, p. 281)

$$J_2 = \frac{16}{\pi^2 v} \int_{-\infty}^{\infty} g(\xi) d\xi \int_{-\infty}^{\infty} \exp(i\rho\eta) d\eta d\zeta \left[1 + \left(\xi + \frac{1}{2} v \right)^2 + \eta^2 + \zeta^2 \right]^{-2} \left[1 + \left(\xi - \frac{1}{2} v \right)^2 + \eta^2 + \zeta^2 \right]^{-2},$$

where

$$g(\xi) = K_0(\rho|\xi|) - K_0(\rho\sqrt{4 + \xi^2}) - \frac{2\rho}{\sqrt{4 + \xi^2}} K_1(\rho\sqrt{4 + \xi^2}).$$

We break up the integrand into simpler fractions and carry out a change of variables. We then obtain

$$J_2 = \frac{32}{\pi v} \int_{-\infty}^{\infty} g(\xi) d\xi \int_0^{\infty} J_0(\rho r) \left\{ \frac{1}{(2v\xi)^2} [1 + (\xi + \frac{1}{2} v)^2 + r^2]^{-2} + [1 + (\xi - \frac{1}{2} v)^2 + r^2]^{-2} + \frac{2}{(2v\xi)^3} \left[[1 + (\xi + \frac{v}{2})^2 + r^2]^{-1} - [1 + (\xi - \frac{v}{2})^2 + r^2]^{-1} \right] \right\} r dr,$$

from which (see reference 11, p. 260) we arrive at the final formula (7).

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