Transfer of angular momentum to Rydberg atoms by charged particles

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The total cross section for transitions from a Rydberg state can be described by a normalized Born approximation when the velocity of the external charged particle is higher than the average velocity of an atomic electron. The discrepancy with experimental data at lower velocities can be eliminated by a more complicated approach based on strong-coupling methods. The methods which have been developed predict that transitions with $|l-l_0|>1$ (l_0 and l are the angular momenta of the initial and final states) will play a dominant role at low velocities. An approximating expression is derived for the total cross section for transitions. Calculations are carried out by the strong-coupling methods for the transitions $28d$–$28f$, $28d$–$28g$, and $28d$–$28h$ in the Na atom.

1. INTRODUCTION

The advances in experimental research on Rydberg atoms have made it possible to detect excited states with very high values of the principal quantum number n ($n\approx 600$ according to Refs. 1 and 2). For such states, the cross sections for the scattering of charged particles are typically extremely large, considerably larger than the orbital area of an atomic electron $\pi a_0^2 n^4$, where $a_0 = 0.53\cdot 10^{-8}$ cm is the atomic unit of length. In order to describe transitions between such states it is necessary to take an approach by which it is possible to find the transition cross sections for arbitrary n. This requirement severely limits the possibilities of the conventional methods of the theory of electron-atom collisions, which have been developed primarily for low-lying excited states.

Our pupose in the present paper is to study the cross sections for the transitions $nl_0 \to nl$ in collisions with charged particles, where l_0 and l are the angular-momentum quantum numbers of the atomic electron in the initial and final states, respectively. The Born approximation[3,4] can be used at high velocities of the charged particles, $v \gg v_0$, where $v_0 = 2.19\cdot 10^8$ cm/s is the atomic unit of velocity. An expression for the cross sections for transitions with $|l_0 - l| = 1$ was derived in Ref. 5 by semiclassical methods. At present the only experimental data available are on the total cross sections for transitions from nd levels in the Na atom.[6] At velocities $v > v_n$ ($v_n = v_0/n$ is the average velocity of an atomic electron), the total cross section is dominated by the transition $d \to f$, and in this case there is a satisfactory agreement between the results of Refs. 5 and 6. At lower velocities, the results derived in Ref. 5 are lower than the experimental results.

In the present paper we show that a modification of the Born approximation to incorporate a normalization effect[7–9] also leads to a satisfactory agreement with experimental data at velocities $v > v_n$. More complicated methods become necessary at velocities $v < v_n$.

Below we report the results of a solution of the strong-coupling equation with a dipole potential for a large number of levels. The total cross sections (for all l) agree with the experimental results over the entire energy range. Furthermore, it follows from our results that transitions with $\Delta l > 1$ become progressively more important in the total cross section with decreasing velocity of the charged particle, becoming the dominant case at velocities $v \lesssim 0.5 v_n$. From the standpoint of studying the basic physics of the collision process, we are particularly interested in approximate models which conserve the basic qualitative features but which allow us to make substantial progress toward an analytic solution of the problem. In particular, it turns out that the total cross section in the energy range of interest here can be described adequately by considering only three levels.

We make no claim that the three-level model is capable of describing transitions with various values of Δl. Demkov and Ostrovskiĭ[10] have derived an expression for the transition probability for the hydrogen atom in terms of a finite-rotation matrix of rank n. In the present paper we examine methods which are based on models with an infinite number of l levels. A distinctive feature of this problem (which contrasts it with, for example, processes involving a change in n) is the lower limit on l. This "semi-infinite" system of equations has been used to derive analytic expressions for the probabilities of transitions with $\Delta l > 1$. [We will use atomic units, expressing the energies in rydbergs (Ry).]

2. BORN APPROXIMATION

The q representation is the most convenient for this analysis of scattering in the Born approximation. In this representation (see Ref. 8, for example) the cross section for the transition $nl_0 \to nl$ is

$$\sigma(nl_0, nl) = \sum_{\varkappa} \sigma_{\varkappa}(nl_0, nl),$$

$$\sigma_{\varkappa}(nl_0, nl) = \frac{8\pi}{v^2}(2\varkappa+1)(2l+1)\begin{pmatrix} l_0 & l & \varkappa \\ 0 & 0 & 0 \end{pmatrix}^2 \int_{k_0-k}^{k_0+k} \frac{dq}{q^3} |R_{\varkappa}(q)|^2, \tag{1}$$

$$R_{\varkappa}(q) = \int_0^{\infty} P_{nl_0}(r) P_{nl}(r) j_{\varkappa}(qr)\, dr,$$

$$k_0 \pm k = (ME_0)^{1/2} \pm [M(E_0 - \Delta E)]^{1/2}, \quad |l_0 - l| \leqslant \varkappa \leqslant |l_0 + l|.$$

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Here ΔE is the transition energy, P_{nl} is the radial wave function, M and E_0 are the mass and energy of the incident particle, and $j_\varkappa(qr)$ is the spherical Bessel function. The general expression for $R_\varkappa(qr)$ is quite complicated, but for the case in which we are interested here, with $n \gg 1$ and $\varkappa = \Delta l$, which dominates the sum over $\varkappa$, the following expressions were derived in Ref. 4 by means of an asymptotic Tricomi expansion for the hypergeometric functions[11] and the Poisson representation for $j_\varkappa(z)$:

$$R_{2m}(q) = \varepsilon_{2m} j_m(qn^2) J_m(qn^2),$$
$$R_{2m+1}(q) = \varepsilon_{2m+1} j_m(qn^2) J_{m+1}(qn^2), \qquad (2)$$
$$\varepsilon_k = \left\{ \prod_{i=0}^{k-1} \left[1 - \left(\frac{l-i}{n} \right)^2 \right] \right\}^{1/2}, \quad l > l_0, \quad m \geqslant 1,$$

where J_m is a Bessel function. These expressions incorporate the equations of Ref. 12 as the limiting case for $l \ll n$. Numerical calculations show that expressions (2) are accurate within a few percent over the important region of qn^2 even at $n > 3$, for nearly all l except $l \sim n$. Using expressions (2), we can write the cross section at $v^2 \gg \Delta E$ as

$$\Delta l = 1: \quad \frac{\sigma(l_0, l_0 \pm 1)}{\pi n^4} = 6 \frac{\max(l_0, l_0 \pm 1)}{2l_0 + 1} \frac{\varepsilon_1^2}{v^2} \mathscr{E}_1 \left(0{,}5 \alpha n^2 \frac{\Delta E}{v} \right),$$
$$\Delta l > 1: \quad \frac{\sigma(l_0, l_0 \pm \Delta l)}{\pi n^4} = 8(2\Delta l + 1)[2(l_0 \pm \Delta l) + 1] \qquad (3)$$
$$\times \begin{pmatrix} l_0 & l_0 \pm \Delta l & \Delta l \\ 0 & 0 & 0 \end{pmatrix}^2 \frac{\varepsilon_{\Delta l}^2}{v^2} K_{\Delta l} (\Delta l)^{-4},$$

where

$$\mathscr{E}_1(z) = \int_z^\infty \frac{dt}{t} e^{-t},$$

and α and $K_{\Delta l}$ are constants found from the numerical calculations: $\alpha = 0.586$, $K_{\Delta l} = 0.454$, 0.422, 0.441 and 0.405 for $\Delta l = 2$, 3, 4, and 5, respectively. It follows from (3) that the cross section falls off rapidly with increasing Δl, and the total cross section for transitions from the nl_0 level is dominated by the dipole cross section, $\Delta l = 1$. Since the only experimental data available at present are on the total cross sections, we will focus below on the dipole transitions, with $\Delta l = 1$. Figure 1 compares the total cross section

$$\sum_{l > 2} \sigma(28d \to 28l)$$

from expression (3) calculated for the Na atom[1)] (this cross section is actually determined by the dipole transition, as we have just seen) with experimental data from Ref. 6. We might note here that calculations from expression (3) yield results which are essentially the same as the dipole Born cross sections calculated in Ref. 3. We see that the Born cross section overestimates the result and that, as expected, for transitions between highly excited states the Born approximation is good only if the dimensionless velocity of the perturbing particle satisfied $x = v/v_n \gg 1$.

To pursue the analysis we also need an expression for the Born cross section for a dipole transition in the impact-parameter representation[5,7] [as usual, we assume a rectilinear trajectory for the perturbing particle, $\mathbf{R}(t) = \boldsymbol{\rho} + \mathbf{v}t$]:

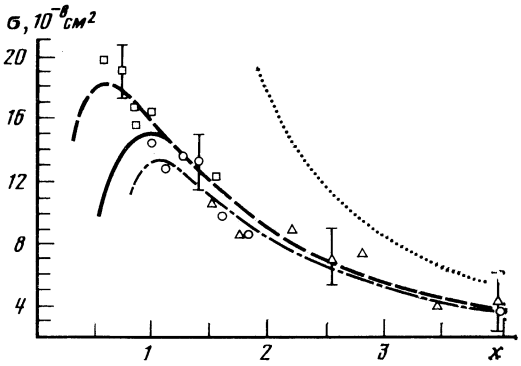

FIG. 1. Cross sections for transitions from the $28d$ state of Na according to perturbation theory ($x = nx/v_0$). The points are experimental data from Ref. 6 on the total cross section for $28d \to 28l$ transitions with $l > 2$. □—Ar^+; ○—Ne^+; △—He^+. Dot-dashed line—Semiclassical calculation[5] of the cross section $d \to f$; dashed line—Born approximation, (3). Normalized Born approximation: Solid line—q representation, (6); dashed line—ρ representation, (4), (5).

$$\sigma_{l_0, l_0 \pm 1} = 2\pi \int_0^\infty W_B(\rho, v) \rho \, d\rho, \quad W_B(\rho, v) = \left(\frac{2\bar{d}}{\rho v} \right)^2 \xi(\beta),$$
$$\xi(\beta) = \beta^2 [K_0^2(\beta) + K_1^2(\beta)], \quad \beta = \omega\rho/v,$$
$$\bar{d} = \left[\frac{1}{2l_0 + 1} \sum_m |\langle n, l_0, m | z | n, l_0 \pm 1, m \rangle|^2 \right]^{1/2} \qquad (4)$$
$$= \frac{\sqrt{3}}{2} \left(\frac{l_>}{2l_0 + 1} \right)^{1/2} n^2 \varepsilon_1,$$

where K_0 and K_1 are modified Hankel functions; ω is the frequency of the transition between the levels l_0, $l_0 \pm 1$ and $l_> = \max\{l_0, l_0 \pm 1\}$.

The Born approximation is valid for weak interactions: at large values of ρ in the ρ representation or at small values of q in the q representation, at which the transition probability is small. If we wish to apply the Born approximation to the cross section as a whole, the region of weak interactions must obviously dominate the cross section for the process. According to the Born approximation, the region of strong interactions frequently makes disproportionately large contributions because the Born transition probability satisfies $W_B > 1$. Consequently, we can significantly expand the range of applicability of the Born approximation if the region of the parameters ρ (or the momenta q) in which the interaction is strong ($W_B > 1$) is eliminated from consideration, or if we arbitrarily set the transition probability in this region at a value less than 1. In the ρ representation, for example, we can determine the transition probability from

$$\overline{W}_B(\rho, v) = W_B(\rho, v) / [1 + W_B(\rho, v)]. \qquad (5)$$

In the q representation, an analogous procedure is carried out as follows ($l = l_0 \pm \Delta l$):

$$\bar{f}_{\Delta l}(q) = |f_{\Delta l}(q)| \left[1 + \frac{q^4}{v^2} |f_{\Delta l}(q)|^2 \right]^{-1/2},$$
$$|f_{\Delta l}(q)| = 2[(2\Delta l + 1)(2l + 1)]^{1/2} \begin{pmatrix} l_0 & l & \varkappa \\ 0 & 0 & 0 \end{pmatrix} |R_{\Delta l}(q)| q^{-2}, \qquad (6)$$

TABLE I. Cross sections for $28d \to 28l$ transitions and the total cross section σ_t in the Na atom for transitions caused by collisions with charged particles

$\frac{\sigma}{\pi a_0^2 n^4} \cdot 10^4$	$x=0,5$		$x=1$		$x=2$	
	(8)	(9), (10)	(8)	(9), (10)	(8)	(9), (10)
$d \to f$	0,094	0,080	0,223	0,202	0,152	0,141
$d \to g$	0,124	0,115	0,069	0,075	0,017	0,018
$d \to h$	0,100	0,152	0,025	0,043	0,005	0,009
σ_t	0,318	0,347	0,317	0,320	0,174	0,168

Note. $x = nv/v_0$. (8)—system of equations with m components; (9), (10)—"average" system, incorporating the d, f, g, and h levels.

where[13]

$$\sigma = \frac{1}{v^2} \int d^2\mathbf{q} |\bar{f}(q)|^2.$$

For the case $\Delta l = 1$, the normalized cross sections calculated from (5) and (6) can be written in the form $\sigma = N\sigma^B$, where σ^B is given by (4), and N can be approximated by

$$N \approx \ln\left[\frac{1+(v^2/v_1v_2)^2}{1+(v/v_2)^2}\right] \Big/ \ln\left(\frac{v}{v_1}\right)^2, \qquad (7)$$
$$v_1 = (\alpha/2)n^2\Delta E, \quad v_2 = (2/\alpha)(\bar{d}/n^2).$$

The overall error of approximation (7) for both representations of the region is less than 20%.

Figure 1 shows Born cross sections for the transition from the $28d$ level, normalized in the ρ and q representations. We see that these cross sections give a satisfactory description of the experimental data at velocities down to $v \sim v_n$.

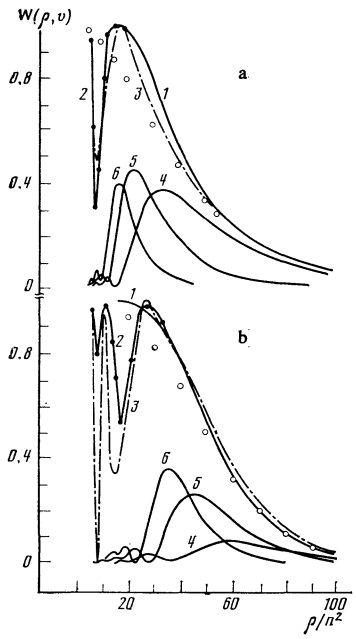

FIG. 2. Probabilities for transitions from the $28d$ state of Na. Strong coupling: a—$x = nv/v_0 = 1$; b—$x = 0.5$. Total probabilities for transitions from the $28d$ level: 1—Complete system, (9), (10), with 26 levels; 2—(dashed line) three-level system, (11); 3—analytic solution, (12), (13); open circles—normalized Born approximation, (4), (5). Probabilities for the transitions $28d \to 28l$ [according to (9), (10), with 26 levels]: 4—$d \to f$; 5—$d \to g$; 6—$d \to h$.

3. STRONG-COUPLING METHOD

Let us examine the strong-coupling method for the transition of an atom from the nl_0 state to the nl state ($l > l_0$). We use the ρ representation. The cross sections for these processes are dominated by the region of large distances between the perturbing particle and the atom: $\rho \gg n^2$. We will thus consider only the dipole interaction, which is dominant at such distances. Since the energy splitting of the levels decreases rapidly with increasing l, we will ignore the energy difference between the level $l_0 + 1$ and the states $l > l_0 + 1$. The strong-coupling system is then[2)] (ω is the frequency of the transition between the l_0 level and the other levels, $l > l_0$)

$$i\dot{a}_{l_0,m}(t) = \sum_{m'} e^{-i\omega t} V_{l_0,m;l_0+1,m'} a_{l_0+1,m'}(t), \quad |m| \leqslant l_0,$$

$$i\dot{a}_{l_0+1,m}(t) = \sum_{m'} e^{i\omega t} V_{l_0+1,m;l_0m'} a_{l_0,m'}(t) + \sum_{m'} V_{l_0+1,m;l_0+2,m'} a_{l_0+2,m'}(t), \quad |m| \leqslant l_0+1,$$

$$i\dot{a}_{l,m}(t) = \sum_{m'} V_{l,m;l-1,m'} a_{l-1,m'}(t) + \sum_{m'} V_{l,m;l+1,m'} a_{l+1,m'}(t), \quad l > l_0+1, \quad |m| \leqslant l, \qquad (8)$$

$$V_{l,m;l'm'} = \delta_{l',l\pm1}\{\langle l, m|z|l', m'\rangle \rho\delta_{m,m'} + \langle l, m|x|l', m'\rangle vt\delta_{m\pm1,m'}\}R^{-3}(t),$$

$$\langle l, m|z|l', m\rangle = \left[\frac{l_>^2 - m^2}{(2l_>+1)(2l_>-1)}\right]^{1/2} R_{n,l}^{n,l\pm1},$$

$$R_{n,l}^{n,l\pm1} = \frac{3}{2}n^2\varepsilon_1,$$

$$\langle l, m|x|l'm'\rangle = \frac{1}{2}\mu\nu\left[\frac{(l_>+\nu+\mu\nu m)(l_>+\mu\nu m)}{(2l_>+1)(2l_>-1)}\right]^{1/2} R_{n,l}^{n,l\pm1},$$

$$\mu = \mathrm{sgn}(m'-m), \quad \nu = \mathrm{sgn}(l'-l).$$

System (8) should be solved under the initial condition

$$|a_{l,m}(-\infty)| = \delta_{l,l_0}\delta_{m,m_0}$$

and then averaged over m_0. Even at small values of n, there are many equations in (8). The dependence on m is not of major importance in this problem. We will accordingly study the system of equations "averaged over m":

$$i\dot{a}_{l_0}(t) = e^{-i\omega t} V_{l_0,l_0+1} a_{l_0+1}(t),$$
$$i\dot{a}_{l_0+1}(t) = e^{i\omega t} V_{l_0+1,l_0} a_{l_0}(t) + V_{l_0+1,l+2} a_{l+2}(t), \qquad (9)$$
$$ia_l(t) = V_{l,l-1} a_{l-1}(t) + V_{l,l+1} a_{l+1}(t)$$

with the initial condition $|a_l(-\infty)| = \delta_{ll_0}$ and the "average" potential

$$V_{l,\,l\pm1}(t) = \bar{d}(\rho+vt)(\rho^2+v^2t^2)^{-3/2}, \qquad (10)$$

where $\bar{d}$ is defined by (4). This expression for the potential gives a qualitatively correct description of the interaction at large distances, and a first-order perturbation-theory treatment of system (9) with potential (10) gives the exact Born expression for the transition probability. To illustrate the situation, we show in Table I the cross sections for transitions from the $28d$ level of *Na* which have been calculated from the complete system (8) and from average system (9), (10) for four values of l. The difference between the results is seen to be insignificant for the total cross section and for the cross section for the transition $d \to f$, while for $d \to g$ and $d \to h$ system (9), (10) still describes the basic qualitative features. Below we will use the average system (9), (10), which is simpler.

Figure 2 shows the probabilities for $28d \to 28l$ transitions versus the impact parameter ρ for velocities $v = v_n$ and $v = (1/2)v_n$ of the external particle according to a solution of system (9), (10) for all $l \geqslant d$ (26 levels). We see that in the region of impact parameters which dominates the cross section the normalized Born approximation for the $d \to f$ transition actually describes not the transition $d \to f$ but the total probability for transitions from the d level. At large values of ρ, as expected, the probability for the transition $d \to f$ which is found from system (9), (10) agrees with the Born probability. We also see that in the region $\rho \lesssim 30n^2$, where the dipole interaction is still dominant, the probability for transitions with $\Delta l > 1$ exceeds the probability for the direct transition $d \to f$. It should be noted that the relative importance of transitions with $\Delta l > 1$ in the overall probability increases with decreasing v.

Figure 3 shows the cross sections for the transitions $d \to f$, $d \to g$, and $d \to h$ for $n = 28$ versus the velocity, in comparison with the total cross section from experiments. Over the entire energy range which has been studied experimentally, the total cross section calculated from system (9), (10) agrees with the data of Ref. 6. At low velocities, however, the total cross section is dominated by transitions with $\Delta l > 1$. In particular, at $v = 0.5v_n$ the cross section for the transition $d \to g$ is greater than that for the transition $d \to f$. Shown for comparison in Fig. 3 is the Born cross section for the transition $d \to g$; we see that it can be ignored.

We can also show that the total transition probability (for all Δl) down to velocities $x \geqslant 0.3$ can be described by simply a three-level system, and we will give an approximate analytic solution for this system. Let us consider a system consisting of the three levels l_0, $l_0 + 1$, and $l_0 + 2$. Diagonalizing the interaction with respect to the levels $l_0 + 1$ and $l_0 + 2$ by means of the transformation

$$|0\rangle = l_0, \quad |-\rangle = \frac{1}{\sqrt{2}}(-|l_0+1\rangle + |l_0+2\rangle),$$

$$|+\rangle = \frac{1}{\sqrt{2}}(|l_0+1\rangle + |l_0+2\rangle)$$

and ignoring the difference between $V_{l_0,\,l_0+1}$ and $V_{l_0+1,\,l_0+2}$, we an rewrite (9) as follows, introducing the dimensionless distance $\tau = vt/\rho$ and the parameter $\lambda = \bar{d}/\rho v$:

$$\begin{aligned} i\dot{a}_0(\tau) &= 2^{-1/2}V(\tau)\{-a_-(\tau)\exp[-i\Phi_-(\tau)] \\ &\quad + a_+(\tau)\exp[-i\Phi_+(\tau)]\}, \\ i\dot{a}_+(\tau) &= 2^{-1/2}V(\tau)\exp[i\Phi_+(\tau)]a_0(\tau), \qquad (11) \\ i\dot{a}_-(\tau) &= -2^{-1/2}V(\tau)\exp[i\Phi_-(\tau)]a_0(\tau), \end{aligned}$$

$$\Phi_\pm(\tau) = \int_0^\tau \alpha_\pm(\tau')d\tau', \quad \alpha_\pm(\tau) = \beta \pm V(\tau),$$

$$V(\tau) = \lambda\frac{1+\tau}{(1+\tau^2)^{3/2}}.$$

This system describes the interaction of the $|0\rangle$ level with the levels $|+\rangle$ and $|-\rangle$, which do not interact with each other.

The total probability for transitions from the $28d$ level found through a numerical solution of system (11) is shown in Fig. 2. In the ρ region which dominates the cross section, this probability is essentially equal to the corresponding probability found from (9), (10).

An approximate analytic solution of system (11) using an asymptotic expansion in the parameter λ was derived in Ref. 14. It can be described by

$$W_t = W_1 + W_2, \quad W_{1,2} = w_\mp(1-w_\pm)/P,$$

$$P = w_+(1-w_-) + w_-(1-w_+) + (1-w_-)(1-w_+), \qquad (12)$$

$$w_\pm = \sin^2\left|\int_{-\infty}^{\infty} d\tau\frac{V(\tau)}{\sqrt{2}}\exp\left\{i\int_0^\tau d\tau'[\alpha_\pm^2(\tau')+2V^2(\tau')]^{1/2}\right\}\right|,$$

where W_t is the total probability for transitions from the d

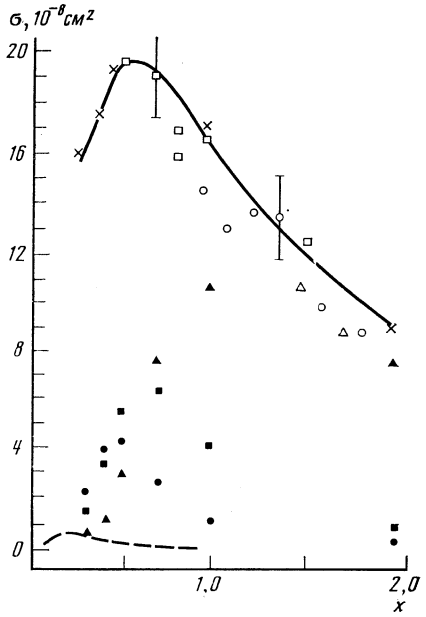

FIG. 3. Cross sections for transitions from the $28d$ state of Na (strong coupling). Total cross section for transitions $28d \to 28l$ with $l > 2$, experimental data of Ref. 6: □—AR^+; ○—Ne^+; △—He^+. Calculations from (9), (10), with 26 levels: ×—Total cross section; ▲—$\sigma_{d\to f}$; ■—$\sigma_{d\to g}$; ●—$\sigma_{d\to h}$. Solid line—Total cross section from (12), (13); dashed line—normalized Born approximation, $\sigma_{d\to g}$.

level, and the probabilities $w_\pm$ are the two-level probabilities for the interaction of only two states. It is a rather difficult matter to evaluate the integrals in (12) for potential (10). An approximate analytic expression for $w_\pm$ which gives results for W_t which agree satisfactorily with the numerical calculations, (11), can be written in the form

$$w_\pm(\rho, v)=\sin^2[{}^1/_2 W_B^{\pm}(\rho, v)]^{1/2}. \tag{13}$$

Here $W_B^{\pm}$ is the Born probability [see (4)], where β is replaced by $\beta_\pm = [(\beta \pm \gamma\lambda)^2 + 2(\gamma\lambda)^2]^{1/2}$, where γ is a parameter of the approximation ($\gamma \approx 0.64$). If $\gamma\lambda > \beta$, we can set $\beta_- = 2^{1/2}\beta$. As can be sen from Fig. 2, the total transition probability found in this manner reproduces quite well the probability found from (9), (10), (11). As a result, the corresponding cross section is essentially the same as that found from complete system (9), (10), and it gives a satisfactory description of the experimental data (Fig. 3).

4. MODELS WITH AN INFINITE NUMBER OF LEVELS

In this section of the paper we consider an analytic approach to the description of the cross sections for transitions with large angular-momentum transfer ($\Delta l > 1$), based on models with an infinite number of levels. Presnyakov and Urnov[15] were the first to propose a model of an unbounded system of equidistant levels, with an interaction potential independent of the level index, for describing transitions between Rydberg levels involving a change in the principal quantum number. In the case of $nl_0 \to nl$ transitions the system of levels which are interacting in the collision process has a lower limit on l, since the energy differences between the levels decrease rapidly with increasing l. We first consider a "semi-infinite" system for levels with identical energies:

$$\begin{aligned} i\dot{a}_k(t) &= V(t)a_{k-1}(t)+V(t)a_{k+1}(t), \quad k>1, \\ i\dot{a}_1(t) &= V(t)a_2(t). \end{aligned} \tag{14}$$

System (14) can be solved in the following way. We add to (14) the complement needed to form the unbounded system:

$$i\dot{a}_k = Va_{k-1}+Va_{k+1}. \tag{15}$$

The solution of system (15) with the initial condition $a_k(-\infty)=\delta_{kk_0}$ (see Ref. 14, for example) is expressed in terms of the generating function Z:

$$a_k(t)=\frac{1}{2\pi}\int_0^{2\pi} e^{-iku}Z_{k_0}(u,t)\,du, \tag{16}$$

$$Z_{k_0}(u,t)=\exp[ik_0u-i\eta(t)\cos u], \quad \eta(t)=2\int_{-\infty}^{t} V(t')\,dt'. \tag{17}$$

It is not difficult to see that if we set

$$Z(u,t)=Z_{k_0}(u,t)-Z_{-k_0}(u,t),$$

then we find a solution of Eq. (15) in which we have $a_0(t)\equiv 0$ and which is thus simultaneously a solution of Eqs. (14).

The solution of system (14) with this initial condition is therefore

$$a_k(t)=\frac{1}{2\pi}\int_0^{2\pi} e^{-iku}[Z_{k_0}(u,t)-Z_{-k_0}(u,t)]\,du, \tag{18}$$

$$Z(u,t)=2i\sum_{k>0} a_k \sin ku, \tag{19}$$

with

$$\sum_{k>0}|a_k(t)|^2=1.$$

We now set $V_{l,l\pm1}=V_{l_0,l_0}\pm 1 = V$ in our "average" system (9). Using (19) for the case $\omega = 0$, and setting $k_0 = 1$, we find the following expression for the amplitudes:

$$\begin{aligned} a_k(\infty) &= i^{1-k}[J_{k-1}(2\lambda)+J_{k+1}(2\lambda)], \\ \lambda &= \frac{\sqrt{3}}{2}\left(\frac{l_0+1}{2l_0+1}\right)^{1/2}\frac{n^2\varepsilon_1}{\rho v}. \end{aligned} \tag{20}$$

More realistic is a model of a semi-infinite system in which, by analogy with (9), one level is separated from the others by a distance $\hbar\omega$:

$$\begin{aligned} &i\dot{b}(t)=V_{ba}(t)a_1(t), \quad i\dot{a}_1(t)=V(t)a_2(t)+V_{ab}(t)b(t), \\ &i\dot{a}_k(t)=V(t)a_{k-1}(t)+V(t)a_{k+1}(t), \\ &V_{ab}(t)=V_{ba}^*(t)=e^{i\omega t}V(t), \quad V(t)=V_{l_0,l_0+1}. \end{aligned} \tag{21}$$

Using the generating function

$$Z(u,t)=2i\sin u\int_{-\infty}^{t} dt' V_{ab}(t')\exp\{i[\eta(t')-\eta(t)]\cos u\}b(t'), \tag{22}$$

we can reduce system (21) to an Volterra integral equation,

$$\begin{aligned} i\dot{b}(t) &= V_{ba}(t)\int_{-\infty}^{t} V_{ab}(t')\mathcal{K}_1(t',t)b(t'),dt', \\ a_k(t) &= \int_{-\infty}^{t} V_{ab}(t')\mathcal{K}_k(t',t)b(t')\,dt', \\ \mathcal{K}_k(t',t) &= 2kJ_k[\eta(t')-\eta(t)]/[\eta(t')-\eta(t)], \quad |b(-\infty)|=1. \end{aligned} \tag{23}$$

Attempts to solve Eq. (23) analytically run into serious difficulties, but Eqs. (23) reduce the infinite system to an integrodifferential system, but for only two levels. For the analysis below it is convenient to rewrite (21) in terms of the function $R(u,t) = Z(u,t)/b(u,t)$:

$$\begin{aligned} i\frac{\partial R}{\partial t} &= 2V(t)R\cos u - V_{ab}(t)2\sin u - iR\frac{\dot{b}(t)}{b(t)}, \\ |b(t)| &= \left[1+\frac{1}{4\pi}\int_0^{2\pi}|R(u,t)|^2\,du\right]^{-1/2}, \\ Z(u,t) &= R(u,t)\left[1+\frac{1}{4\pi}\int_0^{2\pi}|R(u,t)|^2\,du\right]^{-1/2}, \end{aligned} \tag{24}$$

so that the normalization condition

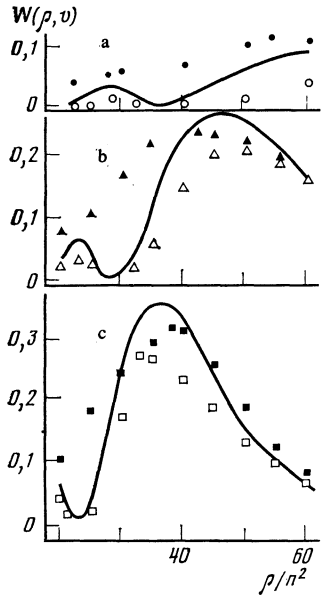

FIG. 4. Probabilities for transitions from the $28d$ state of Na. Models with an infinite number of levels, $x = 0.5$: a—The $d \to f$ transition; b—the $d \to g$ transition; c—the $d \to h$ transition. Filled circles—(25); open circles—(26); solid lines—(9), (10), with 26 levels.

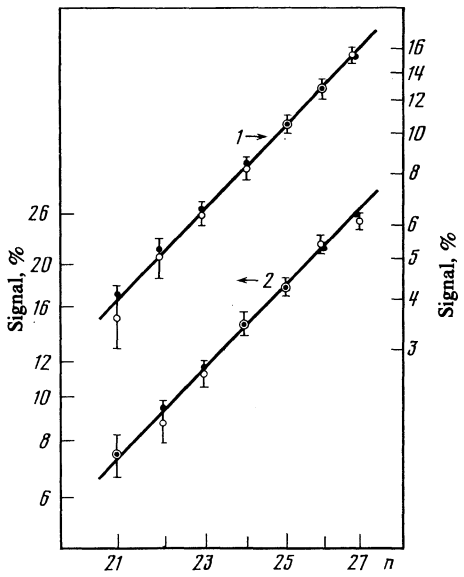

FIG. 5. The total cross section for transitions from the $28d$ level of Na as a function of n. Open circles—Experimental data of Ref. 6; solid lines—mean square experimental dependence[6]; filled circles—present calculations, normalized to the experimental values of the signal[6] at $n = 25$ [Eqs. (3), (7), and (27)].

$$|b|^2+\sum_{k>0}|a_k|^2=1$$

holds independently—regardless of the approximation used in the solution of system (24). In first-order perturbation theory in $V(t)$, we can ignore the term containing $\dot{b}/b$; we find an expression for a_k in closed quadrature form:

$$R(u,\infty)=2i\sin u\int_{-\infty}^{\infty}V_{ab}(t')\exp\{i[\eta(t')-\eta(\infty)]\}dt',$$

$$a_k(\infty)=\frac{b(\infty)}{2\pi}\int_0^{2\pi}e^{-iku}R(u,\infty)\,du, \qquad (25)$$

$$|b(\infty)|=\left[1+\frac{1}{4\pi}\int_0^{2\pi}|R(u,\infty)|^2\,du\right]^{-1/2}.$$

If we set $\eta(t') = 0$ in the integral over t' in (25), we find the following expression for the transition probability from (25):

$$|a_k(\infty)|^2=[(k/2\lambda)J_k(4\lambda)]^2\overline{W}_B(\rho,\nu), \qquad (26)$$

where $\bar{W}_B(\rho, v)$ is the Born probability in (4), normalized in accordance with (5). Figure 4 shows the probabilities for the transitions $d \to l$, $l > 2$ (corresponding to $k = l - 2$) according to (26), in comparison with probabilities found through a numerical integral of (25) and in the finite strong-coupling system, (9), (10). We see, in particular, that at large values of ρ expression (26) leads to an agreement with the results of a solution of system (9), (10), while at small values of ρ the qualitative oscillatory behavior of the probability is preserved. The corresponding cross sections from (26) are smaller than those from (9), (10) by 5–25%, for the most part. The cross sections found from (25) are characterized be the same error, but of the opposite sign.

The probabilities $|a_k(\infty)|^2$ from (26) obviously satisfy the normalization condition explicitly; the total probability for transitions from the b state is $\bar{W}_B(\rho, v)$. Accordingly, if we use a more accurate result [e.g., that which follows from (12), (13)] as the total probability we can thereby refine each transition probability $|a_k(\infty)|^2$.

5. DEPENDENCE OF THE TRANSITION CROSS SECTIONS ON n

At charged-particle velocities above the average velocity of an atomic electron, $v > v_n$, the total cross section for transitions from the nl_0 level is, as we have shown above, described by the normalized Born cross section $\bar{\sigma}(n, l_0; n, l_0 + 1)$ [see (3), (7)]. Figure 5 compares the theoretical and experimental results on the n dependence of the cross sections in the interval 21–28. The n dependence of the cross sections was approximated in Ref. 6 by a function n^α, where $\alpha = 5.41 \pm 0.13$, 504 ± 0.16, and 5.15 ± 0.17 for charged-particle energies of 400, 1000, and 2000 eV, respectively. We see that, within the experimental error, we can assume $\sigma \propto n^2 \ln(Cn)$ in this energy range ($C \approx v^2/\delta$, where δ is the quantum defect of the d state), in accordance with (3) and (7). The difference, however, becomes important in a wider range of n: At $n = 32$, for example, at an energy of 400 eV, the cross section deviates from the power-law approximation by a factor of about 1.3.

The situation at low energies is more complicated. We would obviously like to carry out calculations by the methods developed in Section 3 for each new value of n. In this connection we offer an approximate equation constructed

from (7) and the numerical calculations in accordance with the three-level model for $x \geqslant 0.1$:

$$\sigma = \pi a_0^2 n^4 D \ln\left[1+(x/\delta)^2(1+x_{max}/x)/(D+1)\right], \qquad (27)$$
$$D = 3\frac{l_>}{2l_0+1}\frac{n^2}{x^2} \approx 1{,}5\frac{n^2}{x^2}, \quad l_0 \gg 1,$$

where δ is the quantum defect of level l_0 and $x_{\max} = (n\delta)^{1/2}$ is the estimated position of the maximum of the cross section. At low velocities, $x \ll x_{\max}$, the error of (27) is within a factor of 1.5 or 2, while that near the maximum of the cross section ($x \sim x_{\max}$) is about 20%. At high velocities, expression (27) becomes the Born cross section.

6. CONCLUSION

In sum, the total cross section for transitions from the nl level at high charged-particle velocities can be described by the normalized Born approximation. The discrepancy with experimental data at low velocities is eliminated by a more complicated approach based on strong-coupling methods. The methods developed here predict that transitions with $\Delta l > 1$ will be dominant at low velocities and that the total cross section will fall of (for the d levels of Na, at $v < 0.5v_n$). There is accordingly much interest in seeing further experiments at energies as low as possible and, especially, studying transitions $nl_0 \to nl$ between Rydberg states with an identification of the angular momentum of the final state.

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[1)]The quantum defect of the d levels of Na is 0.011.

[2)]The potential $V_{l,m;l',m'}$ has a pole. This singularity, which is unimportant in the velocity interval under consideration here, leads to a doubling of the cross section at high velocities (see Ref. 12, for example).

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