Impulse-approximation analysis of collisions between Rydberg and ground-state rubidium atoms at thermal energies

I. I. Fabrikant
Department of Physics and Astronomy, University of Nebraska, Lincoln, Nebraska 68588-0111
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The impulse approximation for the Rydberg atom-atom collisions is analyzed on the basis of the Faddeev equations. A modified expression is derived for the cross sections, including the interference between the Rydberg-electron–perturber scattering and the ion-core–perturber scattering. This expression is used for the calculations of the collisional quenching and elastic scattering in Rb(nS)-Rb and Rb(nP)-Rb collisions. We use the electron-Rb scattering phase shifts obtained from *ab initio* close-coupling calculations and their extrapolation, applying the modified effective-range theory. Our results show that the impulse approximation agrees with the experimental data for the quenching cross sections at $n > 20$ but underestimates the quenching cross sections at lower n. The position of the maximum of the cross section is in good agreement with experimental data. We also obtain reasonable results for the elastic cross section at $n > 20$, but for the lower n the results are too large. The interference effect plays a minor role in the process, which means that simultaneous electron-perturber and ion-perturber interaction is unlikely.

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I. INTRODUCTION

The theory of collisions of atoms in Rydberg states with neutral atoms has been developed in great detail for the case when the perturber can be modeled as a source of a very short-range potential (Fermi approximation). This allowed an explanation of the experimental data [1] on collisional depopulation and line broadening of Rydberg atoms when perturbed by rare-gas atoms. In contrast, when the perturber is an alkali-metal atom, the theory is not as well developed. In this case the Rydberg electron-perturber interaction has a very large radius due to both a large polarizability of the perturber, and a low-energy ^3P resonance in electron-perturber scattering. The Fermi approximation was shown [2,3] to be invalid for the principal quantum numbers n up to 50. Two nonempirical calculations [3,4] of the collisional broadening of Rydberg states have been performed which take into account the long-range effects and the ^3P resonance. Fabrikant [3] considered the broadening and shift of Rydberg states in the asymptotic limit of the impulse approximation, which is called the Alekseev and Sobelman theory [5]. More recently the problem of broadening was considered in the adiabatic approximation [4]. This approach permitted us to explain the oscillatory dependence of the width as a function of n as suggested by Borodin and Kazansky [6]. In both cases *ab initio* electron-atom scattering phase shifts were used.

Lebedev and Marchenko [7] calculated the quenching cross sections for Rydberg atoms due to the interaction with Na and Rb atoms employing the impulse approximation, but without using the approximate approach of Alekseev and Sobelman. They used semiempirical scattering phase shifts which were chosen to reproduce experimental data for the quenching cross sections. Also, they did not calculate the contribution of the electron-perturber interaction to the elastic cross sections since it is small compared to the ion-core–perturber contribution at $n > 30$ (the region of principal quantum numbers for which the calculations have been done).

However, the importance of the e-B interaction in elastic A^{**}-B scattering increases rapidly when the principal quantum number decreases. Omont [8] has shown that in the scattering-length approximation the e-B contribution to the elastic cross section varies as $(n^*)^{-4}$, where $n^* = n - \delta$ is the effective principal quantum number, δ being the quantum defect. For the alkali-metal perturbers the e-B interaction becomes important for $n < 30$. In this case the interference between e-B and A^+-B scattering may be essential. One of the major assumptions of the standard impulse approximation is statistical independence of the e-B and A^+-B contributions which implies the condition (atomic units are used throughout the paper)

$$r_{A^+B} \ll n^2 , \tag{1}$$

where $r_{A^+B} = (\pi\alpha/4V)^{1/3}$ is the Weisskopf radius of the polarization interaction, α being the polarizability of the perturber and V the relative A-B velocity. Condition (1) is not satisfied for the alkali-metal perturbers if $n < 30$. Therefore, an investigation of coherence between e-B and A^+-B scattering is important. In order to include this effect, it is useful to rederive the impulse-approximation formulas from the Faddeev equations [9]. This derivation also gives an idea how the impulse approximation might be improved. The Faddeev-Watson expansion [10] has been used by several authors [11–13] for the problem of Rydberg-atom–ground-state-atom collisions in order to estimate the validity of the impulse approximation. Our approach will be close to that of de Prunelé [12], but we will start from the Faddeev equations containing all two-

body interactions rather than from the Faddeev-Watson expansion.

The main purpose of the present paper is an analysis of the impulse approximation and the coherence effect for the Rydberg-atom–alkali-metal-atom collisions for large and intermediate ($15<n<30$) values of the principal quantum number. As an example we have chosen Rb**-Rb collisions because there are quite a few experimental data available on the collisional depopulation [14–16] and collisional self-broadening [2,17] of Rb. On the other hand, the use of the *ab initio* e-Rb scattering phase shifts, obtained from the close-coupling calculations [18] and modified effective-range theory [3], showed good results for the high-n behavior of the collisional widths and shifts [3] and allowed us to explain [4] semiquantitatively the oscillatory dependence of the width as a function of n in the intermediate-n region.

II. FADDEEV EQUATIONS AND THE IMPULSE APPROXIMATION

Let us consider the Rydberg atom A as a system consisting of partices 1 (the ion core A^+) and 2 (the Rydberg electron). This system interacts with a particle 3 (the perturber B). Introduce the Jacobi momentum coordinates

$$\mathbf{k}_{21}=\frac{m_1\mathbf{k}_2-m_2\mathbf{k}_1}{m_1+m_2}\ ,$$
$$\mathbf{q}_3=\frac{(m_1+m_2)\mathbf{k}_3-m_3(\mathbf{k}_1+\mathbf{k}_2)}{m_1+m_2+m_3}\ . \tag{2}$$

The Jacobi coordinates with other indices could be obtained by an appropriate interchange.

Introducing the two-particle Faddeev operators T_{ij} and $T^{(ij)}$ [19], we have the following set of equations:

$$T^{(12)}=\tilde{T}_{12}-T_{12}G_0(T^{(13)}+T^{(23)})\ , \tag{3}$$
$$T^{(13)}=-T_{13}G_0(T^{(12)}+T^{(23)})\ , \tag{4}$$
$$T^{(23)}=-T_{23}G_0(T^{(12)}+T^{(13)})\ , \tag{5}$$

where G_0 is the three-body Green's function for noninteracting particles, $\tilde{T}_{12}$ describes the initial bound state of A^+, and e has the form

$$\tilde{T}_{12}(\mathbf{k}_{21},\mathbf{q}_3)=-\delta(\mathbf{q}_3-\mathbf{p})\left[|\varepsilon_i|+\frac{k_{21}^2}{2m_{12}}\right]\phi_{\varepsilon_i}(\mathbf{k}_{21})\ , \tag{6}$$

where $\mathbf{p}$ is the initial momentum of B relative to A, ε_i is the energy of the bound state, m_{12} is the reduced mass (in our case $m_{12}\approx m_2$), and $\phi_{\varepsilon_i}(\mathbf{k}_{21})$ is the initial bound-state wave function in the momentum space.

T_{13} has the form

$$T_{13}(\mathbf{k}'_{31},\mathbf{q}'_2;\mathbf{k}_{31},\mathbf{q}_2;E)=t_{13}(\mathbf{k}'_{31},\mathbf{k}_{31};\varepsilon_2)\delta(\mathbf{q}'_2-\mathbf{q}_2) \tag{7}$$

where

$$\varepsilon_2=E-\frac{q_2^2}{2\mu_2},\quad \mu_2=\frac{m_2(m_1+m_3)}{m_1+m_2+m_3}\ , \tag{8}$$

t_{13} is the t operator for the two-body problem, and E is the total energy. T_{12} and T_{23} are defined in a similar way.

Equations (3)–(5) should be solved for $T^{(12)},T^{(13)},T^{(23)}$. Then the cross section for B-A scattering, accompanied by the transition $f\leftarrow i$ in the target, is

$$d\sigma_{f\leftarrow i}=\frac{p'}{p}(m_{13})^2(2\pi)^4 d\hat{p}'\,|\mathcal{T}^{(1)}_{f\leftarrow i}+\mathcal{T}^{(2)}_{f\leftarrow i}|^2\ , \tag{9}$$
$$\mathcal{T}^{(n)}_{f\leftarrow i}=-\int\Phi^*_f(\mathbf{k}_{21},\mathbf{q}_3)T^{(n3)}(\mathbf{k}_{21},\mathbf{q}_3)d\mathbf{k}_{21}d\mathbf{q}_3\ , \tag{10}$$

where

$$\Phi_f(\mathbf{k}_{21},\mathbf{q}_3)=\phi_{\varepsilon_f}(\mathbf{k}_{21})\delta(\mathbf{q}_3-\mathbf{p}') \tag{11}$$

is the final-state wave function, $\mathbf{p}'$ being the relative momentum in the final state.

Equations (3)–(5) are very difficult to solve if even we know all properties of the two-body operators t_{ij}. When the system (1-2) is the Rydberg atom, a reasonable approximation is to put $T_{12}=0$. This means that we neglect the e-A^+ interaction during the A-B collision, although the momentum distribution of the initial and final states is taken care of by $\tilde{T}_{12}$ and Φ_f. As a result we obtain two equations

$$T^{(13)}=-T_{13}G_0(\tilde{T}_{12}+T^{(23)})\ , \tag{12}$$
$$T^{(23)}=-T_{23}G_0(\tilde{T}_{12}+T^{(13)})\ . \tag{13}$$

These equations are still coupled. It means that during one A-B collision B can experience many collisions with both e and A^+, although e is considered now as a free particle. Neglecting the coupling, we obtain two independent equations

$$T^{(13)}=-T_{13}G_0\tilde{T}_{12},\quad T^{(23)}=-T_{23}G_0\tilde{T}_{12}\ . \tag{14}$$

Equations (14) and (15) are equivalent to the impulse approximation which treats e-B and A^+-B scattering independently. Its derivation from the Faddeev equations (3)–(5) shows how it can be improved. However, even Eqs. (14) give more than the conventional impulse approximation, because after substitution of Eqs. (14) into Eqs. (9) and (10) for the cross section, we obtain the term describing the interference between e-B and A^+-B scattering which is usually omitted in the impulse approximation. In the remaining part of this section we will obtain the explicit form of the inelastic and elastic cross sections, including the interference effect.

From Eqs. (6), (7), and (14) we obtain

$$T^{(13)}(\mathbf{k}_{21},\mathbf{q}_3)=t_{13}\left[\mathbf{k}'_{31},\mathbf{k}_{31};E-\frac{q_2^2}{2\mu_2}\right]\times\phi_{\varepsilon_i}\left[\mathbf{k}_{21}+\frac{m_2}{m_1+m_2}(\mathbf{q}_3-\mathbf{p})\right]\ , \tag{15}$$

where the arguments of the t_{13} operator should be expressed through $\mathbf{k}_{21}$ and $\mathbf{q}_3$

$$\mathbf{k}_{31}=\frac{m_3}{m_1+m_3}\mathbf{k}_{21}+\frac{m_1(m_1+m_2+m_3)}{(m_1+m_3)(m_1+m_2)}\mathbf{q}_3\ , \tag{16}$$

$$\mathbf{q}_2=\mathbf{k}_{21}+\frac{m_2}{m_1+m_2}\mathbf{q}_3 , \tag{17}$$

and $\mathbf{k}'_{31}$ can be obtained by using the equation $\mathbf{q}'_2=\mathbf{q}_2$.

Similarly

$$T^{(23)}(\mathbf{k}_{21},\mathbf{q}_3)=t_{23}\left[\mathbf{k}'_{23},\mathbf{k}_{23};E-\frac{q_1^2}{2\mu_1}\right] \times\phi_{\varepsilon_i}\left[\mathbf{k}_{21}+\frac{m_1}{m_1+m_2}(\mathbf{q}_3-\mathbf{p})\right] \tag{18}$$

where

$$\mathbf{k}_{23}=\frac{m_3}{m_2+m_3}\mathbf{k}_{21}-\frac{m_2(m_1+m_2+m_3)}{(m_2+m_3)(m_1+m_2)}\mathbf{q}_3 , \tag{19}$$

$$\mathbf{q}_1=\mathbf{k}_{21}+\frac{m_1}{m_1+m_2}\mathbf{q}_3 , \tag{20}$$

and $\mathbf{k}'_{23}$ can be obtained from the equation $\mathbf{q}'_1=\mathbf{q}_1$.

Now we substitute these expressions into Eq. (10) and use the following additional conditions.

(1) $m_1,m_3\gg m_2$.

(2) $\mathbf{p},\mathbf{p}'\gg\mathbf{k}_{21}$. This condition means that the relative A-B momentum is much greater than the electron momentum.

(3) $\mathbf{k}_{21}/m_2\gg\mathbf{p}/m_1$. This means that the typical electron velocity is much greater than the collision velocity. Both (2) and (3) are well satisfied for the thermal collisions.

Then we have

$$\mathcal{T}^{(1)}_{f\leftarrow i}=-\int\phi^*_{\varepsilon_f}(\mathbf{k}_{21})t_{13}\left[\mathbf{p}',\mathbf{p};E-\frac{k_{21}^2}{2m_2}\right] \times\phi_{\varepsilon_i}\left[\mathbf{k}_{21}-\frac{m_2}{m_1}\mathbf{Q}\right]d\mathbf{k}_{21} , \tag{21}$$

where $\mathbf{Q}=\mathbf{p}-\mathbf{p}'$ is the momentum transfer,

$$\mathcal{T}^{(2)}_{f\leftarrow i}=-\int\phi^*_{\varepsilon_f}(\mathbf{k}_{21}+\mathbf{Q})t_{23}\left[\mathbf{k}_{21}+\mathbf{Q},\mathbf{k}_{21};E-\frac{p^2}{2\mu_1}\right] \times\phi_{\varepsilon_i}(\mathbf{k}_{21})d\mathbf{k}_{21} . \tag{22}$$

Equations (21) and (22) can be reduced to the standard impulse approximation for the B-A^+ and e-B scattering, respectively, if we use the on-shell reduction of the two-body t operators. This reduction actually consists of two steps. For the t_{13} operator we have to make the following assumptions.

(1) Assume that $p=p'$. This condition is satisfied very well since the momentum transfer Q is small compared to p

(2) Assume that

$$E-\frac{k_{21}^2}{2m_2}=\frac{p^2}{2\mu},\quad \mu=\frac{m_1m_3}{m_1+m_3} . \tag{23}$$

This condition generally cannot be justified since $E=p^2/2\mu+\varepsilon_i,\varepsilon_i<0$.

For the t_{23} operator we have to assume the following.

(1) $|\mathbf{k}_{21}|=|\mathbf{k}_{21}+\mathbf{Q}|$. This condition is less satisfied than the similar condition for the A^+-B scattering. However, since the main contribution to the integral cross section is due to $Q<1/n^2$ [20] and the typical value of k_{21} is $1/n$, this condition is reasonable.

(2) $E-p^2/2\mu=k_{21}^2/2m_2$. Again, this reduction cannot be justified for the same reasons as for the A^+-B scattering.

We see that invalidity of the second on-shell reduction makes the impulse approximation questionable. de Prunelé [12] investigated the error induced by the second on-shell reduction considering a model separable potential. He found that the error associated with this reduction is of the order of A/n, where A is the scattering length. Therefore the on-shell reduction in the impulse-approximation formula is valid if $n\gg A$. For the thermal-energy collisions of Rydberg atoms with the alkali-metal atoms, this condition leads to the same restriction on n as the single-scattering approximation [4,8]

$$n^3\gg\frac{r_{eB}}{2\pi V} , \tag{24}$$

where r_{eB} is the effective radius of the e-B interaction and $V=p/\mu$ is the collision velocity.

After the on-shell reduction, the differential cross section for the $n'l'\leftarrow nl$ transition averaged over m and summed over m' can be written in the form

$$d\sigma_{n'l'\leftarrow nl}=\frac{1}{2l+1}\frac{p'}{p}\mu_1^2d\Omega_{\mathbf{pp}'}\sum_{mm'}\left|\int\phi^*_{\varepsilon_f}(\mathbf{k}+\mathbf{Q})f_{eB}(\mathbf{k}+\mathbf{Q},\mathbf{k})\phi_{\varepsilon_i}(\mathbf{k})d\mathbf{k}+\frac{1}{\mu_1}f_{A^+B}(\mathbf{p}',\mathbf{p})\int\phi^*_{\varepsilon_f}(\mathbf{k})\phi_{\varepsilon_i}\left[\mathbf{k}-\frac{\mathbf{Q}}{m_1}\right]d\mathbf{k}\right|^2 , \tag{25}$$

where $\mathbf{k}\equiv\mathbf{k}_{21}$, and f_{eB}, f_{A+B} are scattering amplitudes.

In the case of inelastic collisions, the A^+-B contribution is very small [21,22] compared to the e-B contribution. An estimate expression [7] based on the dipole approximation for the calculation of the atomic form factor yields $\sigma^{\text{inel}}_{A^+B}<10$ Å^2 for Rb-Rb collisions at $n=30$, which is four orders of magnitude less than the e-B contribution. Therefore we will include only the e-B contribution for inelastic collisions. In this case calculations of the total cross section

$$\sigma^{\text{inel}}_{nl}=\sum_{n',l'}\sigma_{n'l'\leftarrow nl}$$

can be performed using the quasicontinuum approximation and the closure relation for the momentum-space wave functions, as suggested by Lebedev and Marchenko

[7]. Their result is

$$\sigma_{nl}^{\text{inel}}=\frac{\pi}{V^2}\sum_{n'}\frac{1}{(n')^3}\int_{\varepsilon_{\min}}^{\infty}d\varepsilon\,\varepsilon^{1/2}|g_{nl}(\varepsilon)|^2 \times\int_{-1}^{\nu_{\max}}\frac{d\nu}{(1-\nu)^{1/2}}|f_{eB}(\varepsilon,\nu)|^2 , \tag{26}$$

where g_{nl} is the radial part of the electron wave function in the momentum space as a function of $\varepsilon=k^2/2m_2$, $f_{eB}(\varepsilon,\nu)$ is the e-B scattering amplitude as a function of ε and $\nu=\cos\theta$, where θ is the scattering angle, $\varepsilon_{\min}=|\Delta\varepsilon_{n'nl}|/8v^2$, $\Delta\varepsilon_{n'nl}$ being the energy defect for the transition $nl\rightarrow n'$, and $\nu_{\max}=1-2\varepsilon_{\min}/\varepsilon$. The summation in Eq. (26) goes over all hydrogenlike $n'l'$ states $(3<l'\leq n'-1)$ with negligible quantum defects. The contribution of the states with low l' is negligible [7]. However, the case of elastic scattering $n'l'=nl$ should be considered separately. Generally the exact evaluation of the first integral in Eq. (25) is a complicated task. However, in the case of s states the three-dimensional integral can be reduced to a double integral with the result

$$\sigma_{ns\leftarrow ns}=\frac{2\pi\mu_1^2}{p^2}\times\int Q\,dQ\left|G(Q)+\frac{1}{\mu_1}f_{A^+B}(p,Q)F\left[\frac{Q}{m_1}\right]\right|^2 , \tag{27}$$

where

$$G(Q)=\tfrac{1}{2}\int g_{nl}(k')f_{eB}\left[k,\frac{k+Q\mu}{k'}\right]g_{nl}(k)d\mu\,k^2\,dk , \tag{28}$$

$(k')^2=k^2+Q^2+2kQ\mu$, $\mu=\cos\beta$

where β is the angle between $\mathbf{k}$ and $\mathbf{Q}$ and

$$F(K)=\langle n|e^{i\mathbf{K}\cdot\mathbf{r}}|n\rangle \tag{29}$$

is the atomic form factor which can be put equal to 1 if $n^2K=n^2Q/m_1\ll 1$ [20].

III. SCATTERING AMPLITUDES

As soon as the on-shell reduction of the t operators has been made, we need e-B and A^+-B scattering amplitudes. As in Refs. [3,4] we used the first four partial e-Rb scattering phase shifts calculated by the extrapolation of the close-coupling phase shifts [18] down to low energies using the modified effective-range theory [3]. These phase shifts are presented in Fig. 1. The low-energy behavior of the ^3S phase shift is dominated by a virtual state yielding the scattering length $A=-16.9$ a.u. The scattering length for the ^1S scattering is $A=2.03$ a.u., and the low-energy behavior of the ^3P phase shift is dominated by a resonance with the position $\varepsilon=0.023$ eV and width $\Gamma=0.025$ eV [3].

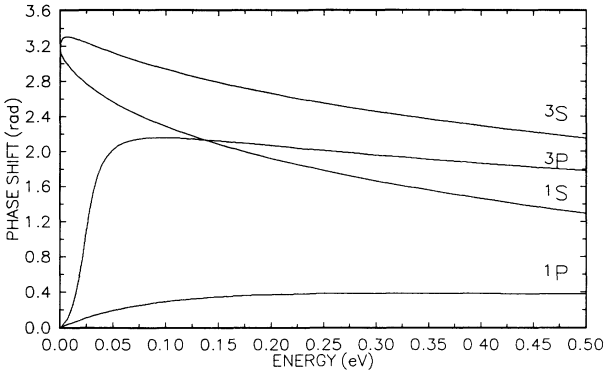

FIG 1. Electron-rubidium scattering phase shifts.

For the calculation of the A^+-B scattering amplitude we used the quasiclassical expression [23] for scattering by the polarization potential $-\alpha/2r^4$

$$f_{A+B}(k,\theta)=\frac{1}{ip}\int_0^{\infty}\lambda(e^{i(g/\lambda^3)}-1)J_0(\lambda\theta)d\lambda , \tag{30}$$

where $g=\pi\alpha\mu p^2/4$ and J_0 is the Bessel function.

If $\theta\gg g^{-1/3}$ integral (30) can be calculated by the stationary-point method with the result [24]

$$f_{A+B}=\frac{(3g)^{1/4}}{2^{1/2}ip\,\theta^{5/4}}\exp[4i(\theta/3)^{3/4}g^{1/4}] \tag{31}$$

and at $\theta=0$

$$f_{A+B}(k,0)=\frac{i}{2p}\Gamma(\tfrac{1}{3})e^{-i\pi/3}g^{2/3} . \tag{32}$$

For $0<\theta\lesssim g^{-1/3}$ integral (30) was calculated numerically.

The scattering amplitude for $\alpha=328$ a.u. (the value used in our calculations) is presented in Fig. 2. The range of angles making the most important contribution to $\sigma_{nS\leftarrow nS}$ lies around $\theta\sim 10^{-3}$, which corresponds to the momentum transfer $Q\sim 10^{-2}$ a.u.

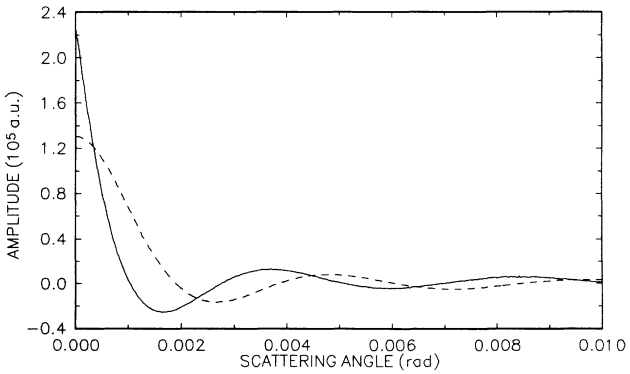

FIG. 2. The real (solid curve) and imaginary (dashed curve) parts of the Rb^+-Rb scattering amplitude. The Rb^+ ion is modeled as a point charge.

IV. RESULTS AND DISCUSSION

In Fig. 3 we present the cross sections for the inelastic Rb(nS)-Rb collisions. Since the quantum defect for the nS states is close to integer ($\delta_0=3.133$), the $n-3\leftarrow n$ transition is dominating. For example, at $n=30$

$$\frac{\sigma_{n-4\leftarrow n}}{\sigma_{n-3\leftarrow n}}=0.0053, \quad \frac{\sigma_{n-2\leftarrow n}}{\sigma_{n-3\leftarrow n}}=0.0019 . \tag{33}$$

At $n\geq 30$ our curve has the same form as the semiempirical curve of Lebedev and Marchenko [7], but gives values which are about a factor of 2 smaller. The same relation is observed between our results and the experimental data [16] in this range of n. However, our results agree much better with the data on collisional broadening which we obtained from Ref. [2] using the relation between the collisional width γ and the total scattering cross section σ

$$\gamma=N\langle V\sigma\rangle , \tag{34}$$

where the angular brackets denote the average over the thermal energy distribution. We also assume that the elastic-scattering contribution to γ is small at large n. In actual calculations we did not perform the averaging over the thermal distribution, but did calculations for two values of V corresponding to the mean velocities $\bar{V}$ at temperatures $T=420$ and 530 K. The velocity dependence of the results appears to be very weak which justifies the approximation

$$\gamma\approx N\bar{V}\sigma(\bar{V}) . \tag{35}$$

At $n\leq 22$ our results are small compared to both sets of experimental data. Apparently, the impulse approximation underestimates the quenching cross sections in this region. Moreover, the elastic contribution becomes significant here, and the disagreement with the broadening data is more essential. It is worth noting that the theoretical results [3] obtained from Alekseev and Sobelman's [5] theory of broadening strongly exceed the experimental data in this region of n and do not give the maximum at $n=23$. The position of the maximum given by the present calculations agrees very well with the experiments. However, the theoretical curve does not show the oscillatory dependence on n in the region of the maximum.

The form of the curve results from the competition between two factors. At large n the probability of e-B collisions becomes less likely due to the large size of the Rydberg atom. At small n the perturber becomes less capable to induce the transitions between nondegenerate ns and $n'l'$ levels because the energy defect $\Delta\varepsilon_{n'nl}$ increases. It could be shown [25] in the scattering-length approximation that the maximum of the quenching cross section appears at $\lambda\approx 1$, where

$$\lambda=\frac{n|\Delta\varepsilon_{n'nl}|}{V} .$$

The position of our maximum agrees quite well with this estimate. It means that the form of the curve $\sigma_{nl}^{\text{inel}}(n)$ is insensitive to the energy dependence of the e-B cross section. For a noticeable influence of the latter on the form of the curve $\sigma_{nl}^{\text{inel}}$ the resonance width should be small compared to the distance between nodes of the momentum-space wave function of the Rydberg electron[3]. This is not the case in our calculations. However, the resonance in the e-B cross section increases the magnitude of the quenching cross section.

To demonstrate these features we also present in Fig. 3 (dashed-dotted curve) results obtained from ^3P phase shifts without the resonant behavior. We assume a bound ^3P state with binding energy 7 meV instead. The curve has essentially the same form as in the case of the resonance, but the magnitude of the cross section is much smaller.

Since at low n the multiscattering effect becomes more important, the impulse approximation in this region underestimates the ability of the perturber to induce the energy transfer. Therefore the calculations give too low values at small n.

In Fig. 4 we present the results for the quenching of

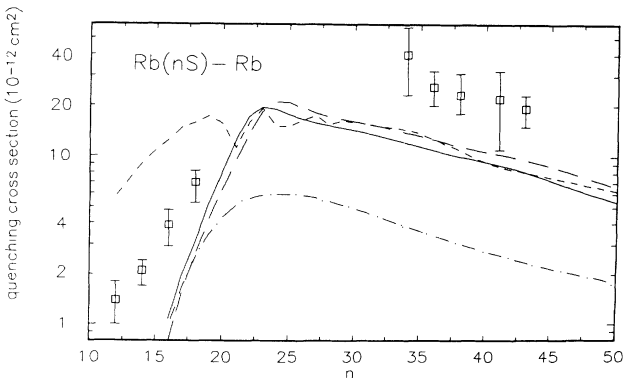

FIG. 3. The quenching cross sections for the Rb(nS)-Rb collisions. Solid curve, calculations for the collision velocity corresponding to $T=530$ K. Long-dashed curve, the same for $T=420$ K. Dashed-dotted curve, cross sections, corresponding to a ^3P bound state of Rb^- with binding energy 7 meV. Short-dashed curve, the total cross sections obtained from the broadening data [2]. Squares with error bars, experimental data [15,16] on the quenching cross sections.

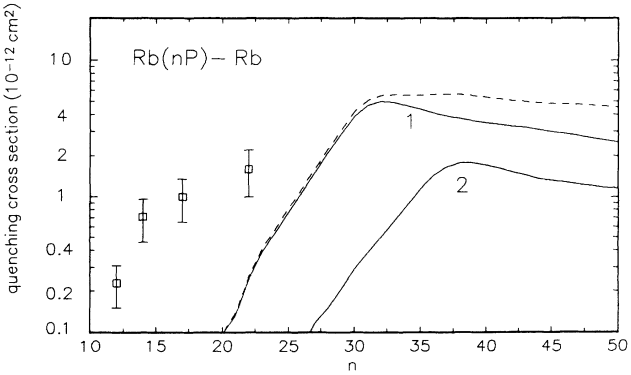

FIG. 4. The quenching cross sections for the Rb(nP)-Rb collisions. Solid curves are contributions due to the $n-3\leftarrow n$ (curve 1) and $n-2\leftarrow n$ (curve 2) transitions. Dashed curve, total theoretical quenching cross sections. Squares with error bars, experimental data [14].

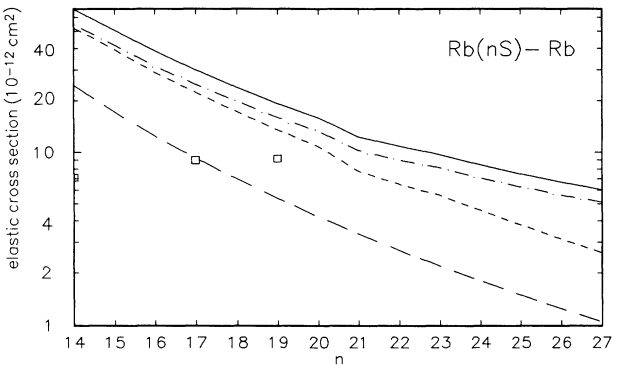

FIG. 5. The elastic cross sections for the Rb(nS)-Rb collisions. Solid curve, total coherent cross section. Short-dashed curve, e-Rb contribution. Dashed-dotted curve, incoherent sum of the e-Rb and Rb^+-Rb contributions. Long-dashed curve, e-Rb contribution calculated in the scattering-length approximation [8]. Squares, "experimental" results obtained from the broadening data [2] and quenching cross-sections data [15] according to Eq. (37).

the nP states of Rb. Experimental data [14] are available only in the low-n region where they strongly exceed the theoretical results. In this case the quantum defect $\delta_1=2.65$ differs substantially from an integer, therefore the contribution of the $n-2\leftarrow n$ transition is nonnegligible.

In Fig. 5 we present the elastic cross sections for the Rb(nS)-Rb collisions in the range of n where the contribution of the elastic scattering is noticeable. Omont's [8] estimate for the e-B contribution to the cross section follows from the scattering-length approximation $f=-A$ and yield

$$\sigma^{\rm el}_{e\text{-}B}=\frac{\pi\overline{A}^2}{V^2(n-\delta)^4}\ , \tag{36}$$

where $\overline{A}^2$ is the square of the scattering length averaged over the spin states for the e-B system. In our case $\overline{A}^2=215.2$.

The proper inclusion of the energy dependence of the scattering amplitude increases the cross section by a factor of 2. The interference between the e-B and A^+-B scattering leads to a further increase of the cross section for the whole range of n values considered, and does not give any nonmonotonical dependence of the cross section on n. It is interesting to note that the coherent A-B scattering cross section exceeds the incoherent sum $\sigma^{\rm el}_{e\text{-}B}+\sigma^{\rm el}_{A^+\text{-}B}$. In order to estimate the relation between the experiment and the theory, we have calculated the "experimental" elastic cross sections at $n=14$, 17, and 19 using the relation

$$\sigma^{\rm el}=\sigma-\sigma^{\rm inel}\ , \tag{37}$$

where the values of σ were taken from the broadening data [2] and those of $\sigma^{\rm inel}$ from the quenching data [15]. This estimate is very crude and may not give reliable results. For example, at $n>30$ the quenching data [16] yield the values which exceed those obtained from the broadening data [2] (see Fig. 3), which means that the experimental errors exceed the elastic-scattering cross section in this region. However, it is reasonable to conclude from Fig. 5 that the impulse approximation overestimates the elastic-scattering cross sections at $n<20$.

V. CONCLUSIONS

We have presented the results of *ab initio* calculations of Rydberg-atom–alkali-metal-atom scattering in the impulse approximation. The impulse approximation gives good results for inelastic cross sections at $n>20$ but underestimates them for lower n values. The elastic-scattering cross sections appear to be too large at $n<20$ in spite of inclusion of the interference between the e-B and A^+-B scattering. Both cross sections do not exhibit an oscillatory dependence on n.

We conclude again that the oscillatory structure of the collisional widths observed in the experiments [2,17] is due to multiple e-B scattering which occurs at low relative A-B velocities [4] not satisfying condition (24). The too low values of our cross sections at low n also are due to neglect of the multiscattering effect. In order to include this effect in the Faddeev equations (3)–(5) we have to leave there the operator T_{12}. As we see from the present results, the simultaneous e-B and A^+-B interaction is very unlikely, therefore we can neglect T_{13} when considering the e-B scattering. As a result we obtain the equation for $T^{(23)}$

$$T^{(23)}=T^{(23)}_{\rm imp}+T_{23}G_0T_{12}G_0T^{(23)}\ , \tag{38}$$

where $T^{(23)}_{\rm imp}$ is the $T^{(23)}$ operator in the impulse approximation. The Faddeev-Watson expansion used by de Prunelé [12] is equivalent to this equation. It will be interesting to compare the solution of this equation for the case of an alkali-metal perturber with the results of Ref. [4] obtained in the adiabatic approximation.

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