Resonances in electron-capture total cross sections for C^{4+} and B^{5+} collisions with H(1*s*)

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Quantal calculations of electron-capture and elastic cross sections have been carried out for collisions of C^{4+} and B^{5+} with H(1*s*) at collision energies $0.00025 < E < 0.02$ eV, where the cross sections show numerous resonances. Positions and widths of the resonances are studied by using the phase-amplitude method.

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I. INTRODUCTION

Electron capture (EC) reactions at low energy are important processes in astrophysical and fusion plasmas. The measurement of the corresponding cross sections is in general carried out by using the merged-beams technique (see Ref. [1]), although these measurements have a limited precision at energies below 1 eV/amu, where the data required in the applications are in general obtained from calculations. EC cross sections at low energies are usually estimated using the Langevin model [2], which assumes an EC probability of 1 for collision energies above the centrifugal barrier, yielding cross sections proportional to $1/\sqrt{E}$. Both detailed calculations [3–5] and experimental results [6] show that the model qualitatively reproduces the increase of the EC cross sections at low energies in collisions of multicharged ions with H, but in general the simple assumption of a transition probability equal to 1 overestimates the EC cross section. In this respect, some attempts have been made (see Refs. [7–9]) to remove this limitation by using the Landau-Zener model [10,11] to estimate the transition probabilities. More serious drawbacks have been found in the calculations of Ref. [12], for elastic scattering and momentum transfer cross sections in $H^+ + H$ collisions, where the Langevin model predicts an incorrect energy dependence. Also recent calculations [5] have pointed out a large isotopic effect in $H^+ +$ Be not predicted by the Langevin model.

On the other hand, it is known (see, e.g., Refs. [4,13,14]) that, for $E < 0.1$ eV/amu, the EC cross section exhibits sharp peaks for systems where the adiabatic potential of the entrance channel has a minimum. In these cases, the effective potentials for the nuclear motion can support several predissociating states for each value of the angular quantum number J. As a consequence, at collision energies near these quasibound states, the EC total cross sections display resonance structures. Although these structures are in general not significant for the calculation of the rate coefficients commonly used in fusion and astrophysics, they are important from a fundamental point of view. In this respect, Rittby *et al.* [13] used a two-state model to evaluate EC cross sections for the $N^{3+} + H(1s)$ collision and assigned the spikes found in their calculation to shape resonances by applying the complex scaling method. Other works [4,14,15] have found similar resonant structures in close-coupling calculations. However, as pointed out in Ref. [9], the main limitation of these calculations is the sensitivity of resonance positions and widths to the quality of the quantum-chemistry calculation applied to evaluate the adiabatic potentials. The recent work of Ref. [16] has shown the presence of Feshbach resonances in the excitation total cross sections in H + Na collisions, and the possibility of measuring orbiting resonances in collisions with cold and ultracold atoms and molecules has been pointed out in Ref. [17].

In the present work, we consider two collision systems: B^{5+} and $C^{4+} + H(1s)$, where two-center wave functions can be accurately calculated. In particular, the molecular wave functions for the quasimolecule BH^{5+} are obtained analytically, and efficient computing codes [18] are available. $C^{4+} + H$ collisions are the prototype of reactions with one effective electron, as the carbon core electrons can be considered as spectators. Also accurate methods are available for evaluating the molecular wave functions and energy curves for this system. It must be noted that several calculations have been carried out for this collision system [3,19–22] which yielded practically identical EC cross sections for energies above 10 eV, although the agreement with the experiments of Refs. [23,24] is less satisfactory, especially at $E < 100$ eV.

The aim of our work is to show the resonant structures that appear in the EC cross sections and quantitatively relate them with the positions and widths of the predissociating states due to the centrifugal barrier of the effective interaction potential. This is carried out by applying the standard technique of Leroy [25] and the phase-amplitude method of Sidkey and Ben-Itzhak [26]. In this respect, we aim to provide a set of data that might be confirmed in merged-beam experiments; in particular, the high-voltage platform of the Oak Ridge National Laboratory will allow high-resolution measurements at low-impact energies [27]. On the other hand, given the growing interest in elastic cross sections for plasma modeling [28], and since calculations on $H^+ + H$ [29,30] and $H^+ +$ inert gases [31] collisions have shown resonant structures in the elastic cross section, we have also considered elastic cross sections for $B^{5+} + H$ and $C^{4+} + H$ collisions. Atomic units are employed unless otherwise stated.

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II. COMPUTATIONAL METHOD

The calculation of EC total cross sections has been carried out by using the method described in previous works [22,32]. It employs a molecular expansion of the collisional wave function, Ψ^J, for each value of the total angular momentum, J, in terms of the molecular functions, ϕ_k:

$$\Psi^J(\boldsymbol{r},\boldsymbol{\xi}) = \sum_k \chi_k^J(\boldsymbol{\xi})\phi_k(\boldsymbol{r},\xi), \tag{1}$$

where the functions ϕ_k are (approximate) eigenfunctions of the clamped-nuclei electronic Hamiltonian, $H_{\rm elec}$,

$$H_{\rm elec}\phi_k(\boldsymbol{r},\xi) = \epsilon_k(\xi)\phi_k(\boldsymbol{r},\xi). \tag{2}$$

The total Hamiltonian of the system is written as

$$H = -\frac{1}{2\mu}\nabla_R^2 + H_{\rm elec} = -\frac{1}{2\mu}\nabla_R^2 - \frac{1}{2}\nabla^2 + U(\boldsymbol{r};R), \tag{3}$$

where R is the internuclear distance, $\boldsymbol{r}$ denotes the electron vector position with respect to the nuclear center of mass, μ is the reduced mass of the colliding system (0.929269 u for $^{12}C^{4+}$-H, 0.923284 u for $^{11}B^{5+}$-H), and U is the electron-nuclei Coulomb potential. In the case of B^{5+} + H collisions,

$$U(\boldsymbol{r};R) = -\frac{5}{r_B} - \frac{1}{r_H}. \tag{4}$$

For C^{4+} + H collisions the electronic Hamiltonian includes a model potential to describe the interaction of the active electron with the $1s^2$ shell. It has the form

$$U(\boldsymbol{r};R) = -\frac{2}{r_C} - \frac{2}{r_C}(1+\beta_1 r_C)\exp(-\beta_2 r_C) - \frac{1}{r_H}, \tag{5}$$

where r_X is the electron distance to the nucleus X, ($X = H,C,B$). The parameters β_1 and β_2 were obtained by fitting the energy levels of C^{3+} (see Ref. [19]), and the accuracy of the potential energy curves and dynamical couplings of CH^{4+}, obtained with this model potential, was checked by comparing them with the corresponding *ab initio* ones in Ref. [22].

In Eq. (1) the molecular wave functions are expressed as functions of a common reaction coordinate (CRC) $\boldsymbol{\xi}(\boldsymbol{r},R)$ to ensure that the expansion fulfills the boundary conditions (see Ref. [33]). In the present calculation the CRC is defined in terms of the switching function of Ref. [34], as explained in detail in Ref. [35]. Substitution of the expansion (1) in the stationary Schrödinger equation leads to a set of differential equations, whose solutions are the nuclear functions χ_k^J. The scattering matrix S^J is then calculated from these nuclear functions, and the total cross section for transition from the state i to the state j is given by

$$\sigma_{ij}(E) = \frac{\pi}{k_i^2}\sum_J (2J+1)\left|\delta_{ij} - S_{ij}^J\right|^2, \tag{6}$$

where E is the collision energy.

At $E < 1$ eV/u, the simplest model to estimate the EC cross section for the two collision systems considered in this work is the Langevin model, where the electronic energies of the entrance channels have the form

$$\epsilon_1(R) \sim -\frac{q^2\alpha}{2R^4}, \tag{7}$$

where $\alpha = 4.5$ is the polarizability of H($1s$) and q the charge of the projectile. The Langevin formula for the EC cross section is obtained by assuming classical nuclear motion in the polarization potential given in Eq. (7). In this model the EC process takes place for those trajectories with values of the impact parameter, b, and energy, $E(=1/2\mu v^2)$, which allow the surmounting of the centrifugal barrier; this yields

$$\sigma_{\rm L}(E) = \pi b_{\rm max}^2 = \pi q(2\alpha/E)^{1/2}, \tag{8}$$

where $b_{\rm max}$ is the maximum impact parameter that allows passage over the centrifugal barrier.

We also include in the illustrations the cross sections obtained by applying the Landau-Zener-Langevin (LZL) model, where the EC cross section is obtained by integrating the EC transition probability given by the Landau-Zener formula,

$$\sigma \simeq 4\pi\int_0^{b_{\rm max}} bp(1-p)db, \quad \text{with} \quad p = \exp\left(\frac{-2\pi H_{12}^2}{a v_r}\right),$$
$$a = \frac{d(H_{22}-H_{11})}{dR}, \quad v_r = v\left(1 - \frac{H_{11}(R_0)}{E} - \frac{b^2}{R_0^2}\right)^{1/2}, \tag{9}$$

and assuming that the EC probability vanishes for $b > b_{\rm max}$, with $b_{\rm max}$ defined as in the Langevin model [see Eq. (8)]. R_0 is the crossing point of the energies of the diabatic states [$H_{22}(R_0) - H_{11}(R_0) = 0$]. In the model of Eq. (9) the potential energy curves, H_{11} and H_{22}, are used to evaluate the transition probability and in particular for the definition of the radial velocity, v_r, while the value of $b_{\rm max}$ is obtained from the polarization potential. We have checked that, for the two systems studied, the total cross sections were indistinguishable from those obtained by using the polarization potential instead of H_{11} in the definition of the radial velocity.

Finally, we also applied the phase amplitude method [26] to determine the centroid and width of each of the tabulated resonances (see Tables I and II for C^{4+} + H($1s$) and B^{5+} + H($1s$), respectively). Briefly, in this method the wave function of any one-dimensional problem is written as a product of a phase, ϕ, and a logarithm of an amplitude, $\gamma(r)$, namely,

$$\psi(R) = \sqrt{2\mu/\pi}\,\exp[\gamma(R)]\sin[\phi(R)]. \tag{10}$$

This leads to the coupled phase-amplitude equations

$$\frac{d^2\gamma}{dR^2} + \left(\frac{d\gamma}{dR}\right)^2 - \left(\frac{d\phi}{dR}\right)^2 + 2\mu[E - V(R)] = 0, \tag{11}$$

$$\frac{d\phi}{dR} = \exp[-2\gamma], \tag{12}$$

which are solved numerically as discussed in detail in Ref. [26]. It is important to note that the accuracy of the solutions is only limited by numerical precision (that one can adjust for the problem at hand) and more importantly by the quality of the potential $V(R)$ used. In our calculation this potential is the eigenvalue of Eq. (2) for the molecular state that adiabatically correlates to the collision entrance channel [the tabulated $V(R)$ is interpolated using a cubic spline]. The corresponding potentials for the two systems considered are shown in Fig. 1.

Resonances are identified by a shift of π in the phase and a peak in the natural logarithm of the phase derivative. The

TABLE I. Comparison of the positions and widths in eV of the EC resonances in $C^{4+} + H(1s)$ collisions obtained by applying the Breit-Wigner (BW) [Eq. (14)] to those of the quasistationary states calculated using the phase-amplitude (PA) method [26] and applying the program LEVEL [25].

v	J	E_r (BW)	Γ (BW)	E_r (PA)	Γ (PA)	E_r (LEVEL)	Γ (LEVEL)
8	13	0.00046	5.5×10^{-5}	0.00050	2.0×10^{-5}	0.00050	3.1×10^{-5}
7	16	0.00108	9.3×10^{-5}	0.00116	5.4×10^{-5}	0.00117	1.1×10^{-4}
6	19	0.00209	1.2×10^{-4}	0.00223	5.8×10^{-5}	0.00223	8.0×10^{-5}
5	22	0.00353	–	0.00373	2.5×10^{-5}	0.00373	2.7×10^{-5}
4	26	0.00727	1.8×10^{-4}	0.00755	1.1×10^{-4}	0.00755	1.5×10^{-4}
3	30	0.01271	2.2×10^{-4}	0.01308	1.6×10^{-4}	0.01309	2.2×10^{-4}
2	34	0.01984	1.5×10^{-4}	0.02039	7.7×10^{-5}	0.02039	7.8×10^{-5}
2	35	0.02374	4.3×10^{-4}	0.02420	5.2×10^{-5}	0.02424	1.0×10^{-3}

resonance energy and width are then determined by fitting a standard Breit-Wigner form plus a constant to the phase derivative, explicitly,

$$\frac{d\phi}{dE} = \frac{\Gamma/2}{(E - E_r)^2 + (\Gamma/2)^2} + \text{constant}, \tag{13}$$

where E_r and Γ are the resonance energy and width, respectively (see Ref. [26] for further details). In Fig. 2 we show, for example, the solution for the $J = 22$ resonance in the $C^{4+} + H(1s)$ collision system.

III. RESULTS

A. C^{4+} + H collisions

The EC reaction takes place through transitions from the molecular orbital $5g\sigma$ to molecular orbitals dissociating into $C^{3+}(1s^2 4l) + H^+$. In particular, at low energies, the entrance channel is depopulated via transitions to the $4f\sigma$ molecular orbital; this is illustrated in Fig. 3, where we compare 2-state ($4f\sigma$,$5g\sigma$) results with those from the 20-state basis set of Ref. [22]. The EC cross section of Fig. 3 shows many resonant structures, including below- and above-the-barrier resonances. We find a larger number of resonances in this cross section than in previous calculations [4] for $N^{2+} + H$ and $O^{2+} + H$ collisions, since, as q increases, the polarization interaction becomes stronger, yielding a deeper potential minimum.

In order to study the origin of the resonances, we have employed the Breit-Wigner expression for the contribution of the Jth partial wave to the total CE cross section,

$$\sigma_r(J) = (2J + 1)\frac{\pi}{k^2}\frac{\Gamma_e \Gamma_r}{(E - E_r)^2 + \frac{1}{4}\Gamma^2}, \tag{14}$$

to obtain the position and width of some of the resonances of Fig. 3. In this expression (see, e.g., Ref. [36]), Γ is the total width of the resonance and Γ_e the elastic contribution to it. $\Gamma_r (= \Gamma - \Gamma_e)$ is the inelastic contribution. We have fitted the peaks of the EC cross section to this expression and the values of E_r and Γ are shown in Table I. The values of Γ_e are smaller than 10^{-9} eV. For comparison we also show the resonance positions and widths computed with the phase-amplitude method, which are in reasonable agreement with the EC calculations. However, the phase-amplitude calculations yield slightly higher resonance energies, by about 0.04–0.5 meV (i.e., 2–8%), and somewhat narrower resonances. We include in Table I the position and widths evaluated using the program LEVEL [25]. In general, the one-channel calculations (phase amplitude and LEVEL) yield resonance positions that differ

TABLE II. Comparison of the positions and widths in eV of the EC resonances in $B^{5+} + H(1s)$ collisions obtained by applying the Breit-Wigner (BW) [Eq. (14)] to those of the quasistationary states obtained by applying the phase-amplitude (PA) method [26] and the program LEVEL [25].

v	J	E_r (BW)	Γ (BW)	E_r (PA)	Γ (PA)	E_r (LEVEL)	Γ (LEVEL)
	25	–	–	0.00478	6.0×10^{-4}	–	–
1	27	–	–	0.00527	6.3×10^{-6}	–	–
1	28	0.00637	9.3×10^{-5}	0.00672	8.8×10^{-5}	0.00668	9.2×10^{-5}
	29	0.00786	5.5×10^{-4}	0.00815	3.6×10^{-4}	–	–
	30	0.00938	1.7×10^{-3}	0.00960	8.2×10^{-4}	–	–
	31	0.0108	2.3×10^{-3}	0.0111	1.5×10^{-3}	–	–
	32	0.0124	3.4×10^{-3}	0.0127	2.3×10^{-3}	–	–
0	34	0.0130	3.2×10^{-5}	0.0132	1.1×10^{-5}	0.0131	6.2×10^{-5}
0	35	0.0155	2.0×10^{-4}	0.0157	7.9×10^{-5}	0.0156	6.5×10^{-5}
0	36	0.0180	4.6×10^{-4}	0.0182	2.7×10^{-4}	0.0181	3.9×10^{-4}
	37	0.0204	1.4×10^{-3}	0.0207	6.1×10^{-4}	–	–
	38	0.0227	1.1×10^{-3}	0.0234	1.1×10^{-3}	–	–
	39	–	–	0.0261	1.7×10^{-3}	–	–

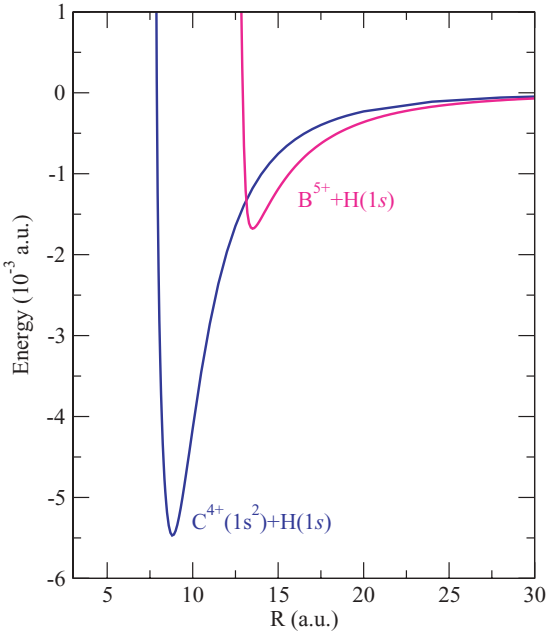

FIG. 1. (Color online) Potential energy curves of the molecular states that dissociate into $C^{4+} + H(1s)$ and $B^{5+} + H(1s)$.

in less than 1%, but the corresponding widths only show qualitative agreement.

For below-barrier resonances, we indicate in Fig. 3 the quantum numbers (v, J) associated with them. For over-barrier resonances only J is indicated. In order to get smooth curves the energy grid employed to plot Fig. 3 is not uniform; we have varied it during the calculation and checked that all resonances obtained with the program LEVEL with $\Gamma \geqslant 5 \times 10^{-6}$ eV are shown.

B. $B^{5+} + H$ collisions

The main mechanism of the EC process involves $5g\sigma$-$4f\sigma$ transitions in the corresponding avoided crossing at $R \simeq 12.9a_0$. In the calculation we have employed a 12-term

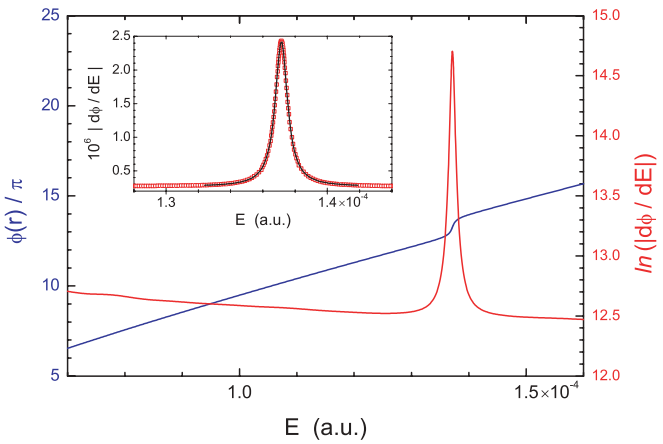

FIG. 2. (Color online) The phase (blue) and natural log of the phase derivative (red) as a function of energy for the $J = 22$ resonance of the $C^{4+} + H(1s)$ collision system. The inset shows a zoomed-in view of the resonance phase derivative as a function of energy and a fit of Eq. (13) to the phase derivative, $d\phi/dE$.

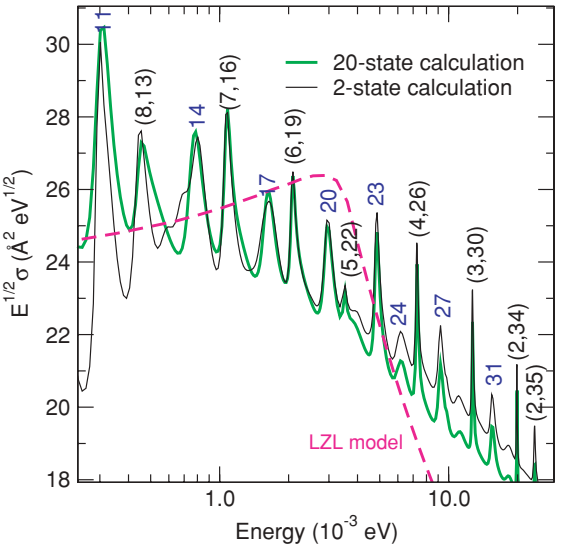

FIG. 3. (Color online) EC cross sections in $C^{4+} + H(1s)$ collisions as functions of the impact energy. The dashed line has been obtained by applying the LZL model of Eq. (9) to the avoided crossing between the energy curves of the σ molecular orbitals that dissociate into $C^{4+} + H(1s)$ and $C^{3+}(1s^2 3d) + H^+$. The values of the quantum numbers (v, J) are indicated for below-barrier resonances and J for over-barrier resonances at the positions of the corresponding peaks in the cross section.

molecular basis set that includes the entrance channel, the molecular orbitals dissociating into $B^{4+}(n = 4) + H^+$ and the $6h\sigma$ orbital, which correlates to $B^{4+}(n = 5) + H^+$. At $R < 12.9a_0$, the adiabatic potential energy curve of the entrance channel increases as $4/R$, and therefore, this potential shows a shallow minimum compared to that of CH^{4+}, and it supports a smaller number of quasibound states. The EC total cross sections for $B^{5+} + H(1s)$ collisions are plotted in Fig. 4, where one can note the relatively large number

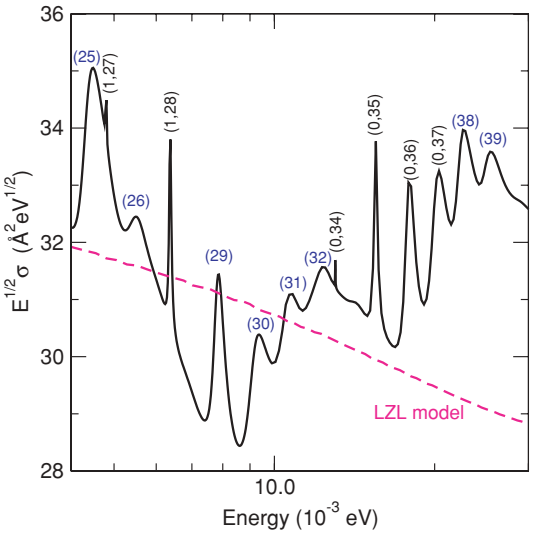

FIG. 4. (Color online) EC cross sections in $B^{5+} + H(1s)$ collisions as functions of the impact energy. The dashed line has been obtained by applying the LZL model of Eq. (9) to the $5g\sigma$-$4f\sigma$ avoided crossing.

of over-barrier resonances. In the phase-amplitude method, over-barrier resonances do not show a shift of π in the resonance region, although the derivative of the phase has a maximum. The corresponding wave functions are similar to scattering waves but with a somewhat higher probability in the region of the well. In Table II we do not give the data for the over-barrier resonances calculated with LEVEL, since they are not routinely obtained with this program. Since the Breit-Wigner fitting of the EC cross section does not provide accurate data for some of the resonances, we have not included them in the table, but the qualitative agreement with the phase-amplitude results, together with the analysis of the S matrix, allows us to assign the values of J shown in Table II and Fig. 4. As for the CH^{4+} system, there is good agreement between the energies of the quasistationary states and the positions of the peaks in the EC cross section, but only the order of magnitude of the corresponding widths is reproduced.

C. Elastic cross sections

The elastic cross section for $C^{4+} + H(1s)$ collisions is shown in Fig. 5. It has been evaluated by including partial waves up to $J = 300$, and we have checked that identical values were obtained when the range was reduced to $J = 150$. We include in this figure the total cross sections evaluated using the 20-state basis set employed in the calculation of the EC cross sections and the corresponding values from a 1-state calculation. Both results show a similar energy dependence, but nonadiabatic transitions lead to a noticeable decrease of the elastic cross sections evaluated with the 20-state basis. Both lines show a similar energy dependence with an oscillatory shape, similar to that found in early calculations [37–40]. To further study the elastic cross section we have carried out a simple JWKB estimate (see, e.g., Ref. [41]), where we have not included tunneling through the centrifugal barrier. The elastic phase shift is then obtained as

$$\eta_J^{SC} = \lim_{R\to\infty}\left\{\int_{R_J}^{R} k_J(R)\mathrm{d}R - kR + \left(J+\frac{1}{2}\right)\frac{\pi}{2}\right\}, \quad (15)$$

where $k = \sqrt{2\mu E}$,

$$k_J(R) = \left[2\mu[E - V(R)] - \frac{\left(J+\frac{1}{2}\right)^2}{R^2}\right]^{1/2}, \quad (16)$$

and R_J is the classical turning point. The total elastic cross section in this simple semiclassical approximation is then given by

$$\sigma_{\mathrm{el}}^{\mathrm{SC}} = \frac{4\pi}{k^2}\sum_{J=0}^{\infty}(2J+1)\sin^2\eta_J^{\mathrm{SC}}. \quad (17)$$

The undulatory structure of the semiclassical cross section is very similar to that of the quantal calculations, and we have also checked that the J dependence of the scattering matrix given by Eq. (17) is also very similar to that obtained numerically. Further insight into the structure of the elastic cross section is obtained by considering the glory contribution to this cross section (see Ref. [41]),

$$\sigma_g = -\frac{2\pi^{3/2}}{k^2}(2J_g+1)\left|\frac{\partial^2\eta_J}{\partial J^2}\right|_{J_g}^{-1/2}\cos\left(2\eta_{J_g} - \pi/4\right). \quad (18)$$

In order to compare with the one-state calculation, we have estimated the nonoscillatory part of the cross section by using the Schiff-Landau-Lifshitz approximation (SLL) [36,42,43] to show that the main oscillatory structure is given by the glory oscillation. We have also found 11 maxima by extending the energy range of the semiclassical estimate

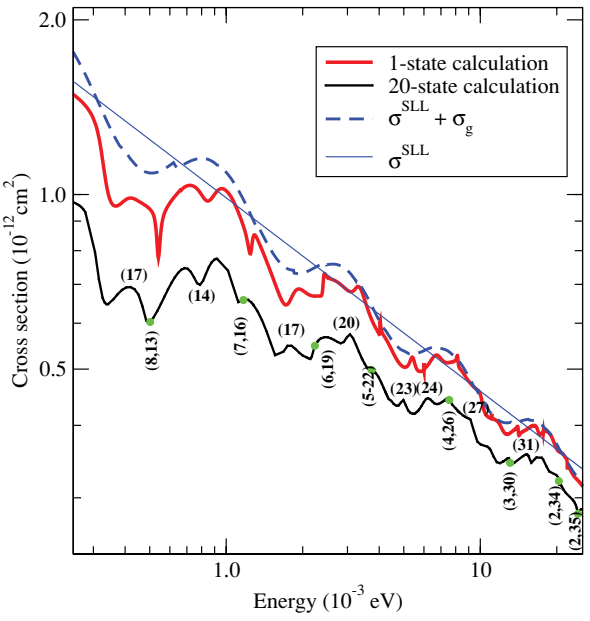

FIG. 5. (Color online) Elastic cross section for $C^{4+} + H(1s)$ collisions as a function of the impact energy. Full lines, quantal calculations. Dashed line, illustration of the glory contribution, σ_g from Eq. (18) and the Schiff-Landau-Lifsihtz (SLL) approximation. The points, labeled (ν, J), indicate the positions of the below-barrier resonances of Table I. The approximate positions of the over-barrier resonances are also indicated.

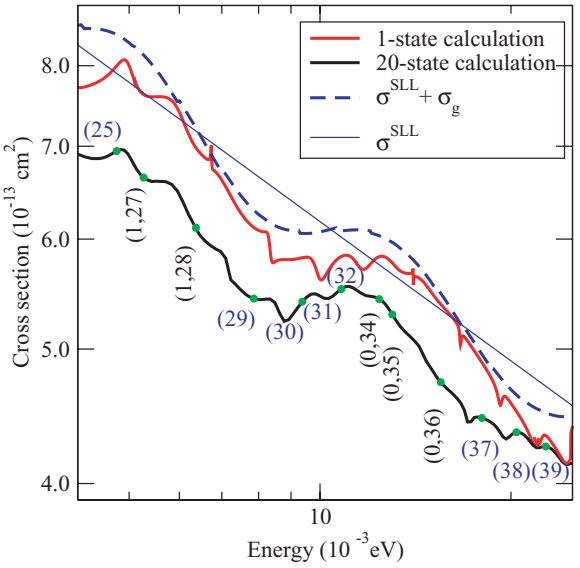

FIG. 6. (Color online) Elastic cross section for $B^{5+} + H(1s)$ collisions as function of the impact energy. Line assignment as in Fig. 5. The positions of the resonances of Table II are indicated on the line that corresponds to the 12-state calculation.

($E > 2.5 \times 10^{-5}$ eV), and the semiclassical phase shift $\eta_0(E = 2.5 \times 10^{-5}\ \text{eV}) = 37.1$ is in agreement with the fact that the potential supports 12 bound states (an additional maximum is located at E lower than those considered). The remaining structures in Fig. 5 are related to resonances, although they are not as clearly observed as in the EC cross section. To illustrate this point, we have indicated in Fig. 5 the positions of the resonances found in the EC cross section of Fig. 3. In particular, over-barrier resonances are related to the most conspicuous structures.

For completeness, we have also calculated the elastic cross section for $B^{5+} + H(1s)$ collisions, which is shown in Fig. 6. As in $C^4 + H$ collisions, the basic structure of the energy dependence of the total elastic cross section is due to glory oscillations and a sizable decrease is obtained when nonadiabatic transitions are allowed. The rotationless potential supports in this case only 9 bound states, and we obtain $\eta_0(E = 2.5\ \text{eV}) = 25.8$.

IV. CONCLUSIONS

We have calculated electron-capture and elastic total cross sections for C^{4+} and B^{5+} using a quantal molecular treatment. We have found several spikes in the EC cross sections, which correspond to shape resonances in the entrance channel adiabatic potential. Some spikes are produced by particular quasibound states of the effective potential and have been assigned the corresponding pair of quantum numbers (ν, J), while other, in general broader structures, correspond to above the barrier resonances and only the rotational quantum number (J) has been assigned to them. The calculation of positions and widths of the quasistationary states, using the phase-amplitude method, quantitatively supports the explanation of the structure of the cross section as due to shape resonances. We have also shown that the EC cross sections oscillate around the estimate of the semiclassical Landau-Zener-Langevin model. The shape of the elastic cross sections clearly show glory oscillations and additional structures can be ascribed to shape resonances at the same energies where we have found resonances in the EC cross section.

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