Crossover of Feshbach Resonances to Shape-Type Resonances in Electron-Hydrogen Atom Excitation with a Screened Coulomb Interaction

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The effects of Coulomb interaction screening on electron-hydrogen atom excitation in the $n = 2$ threshold region are investigated by using the R-matrix method with pseudostates. The interaction screening lifts the l degeneracy of $n = 2$ Coulomb energy level, producing two distinct thresholds for $2s$ and $2p$ states. The phenomenon of transformation of $^{1,3}P$ and ^{1}D Feshbach resonances into shape-type resonances is observed when they pass across the $2s$ and $2p$ threshold, respectively, as the interaction screening increases. It is shown that this resonance transformation leads to dramatic effects in the $1s \rightarrow 2s$ and $1s \rightarrow 2p$ excitation collision strengths in the $n = 2$ threshold collision energy region.

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Screened Coulomb interaction between charged particles appears in many physical systems (hot, dense plasmas, electrolytes, solid-state matter) and profoundly affects the structure and collision properties of composite particles in these systems [1–3]. The Coulomb interaction screening in these systems is a collective effect of correlated many-particle interactions, and in the lowest particle correlation order (pairwise correlations) it reduces to the Debye-Hückel (Yukawa-type) potential. For the interaction of an ion of charge Z with an electron it has the familiar form [1–3]

$$V(r) = -\frac{Ze^2}{r}\exp\left(-\frac{r}{D}\right), \tag{1}$$

where D is the screening length. In a plasma, $D = (k_B T_e/4\pi e^2 n_e)^{1/2}$, with T_e and n_e being the plasma electron temperature and density, respectively, and k_B the Boltzmann constant.

Motivated mainly by the spectroscopic studies of hot, dense plasmas [4], a number of theoretical investigations have been carried out on the plasma screening effects in the electron-hydrogen-like ion excitation [5–9] and ionization [10] collisions by using the potential (1) within the Born [5,7–10] or two-state close-coupling [6] approximations. These papers, however, have not addressed the question of the effects of screened Coulomb interaction on the resonances around the thresholds of inelastic processes.

The purpose of the present Letter is to investigate the Coulomb interaction screening effects on the $1s \rightarrow 2s$ and $1s \rightarrow 2p$ excitation in electron-hydrogen atom collisions in the $n = 2$ resonant energy region by employing the R-matrix method with pseudostates (RMPS). While far from the resonant energy region the Coulomb interaction screening leads generally to reduction of the cross section for a specific process, in the resonant region it leads to dramatic changes both in its magnitude and structure. As it is revealed in the present work, the major effect of the Coulomb interactions screening in the resonant energy region is the transformation of Feshbach resonances into shape-type resonances, which is reflected in dramatic changes in the cross section structure and magnitude with respect to the unscreened case. As we shall see later, this phenomenon has a general nature and is related to the coupling of two-electron states with different angular momentum in the threshold region when the Coulomb interaction is screened and should, therefore, manifest itself in the higher-n threshold excitation regions as well.

As it is well known (see, e.g., [11]), resonances in electron-atom collisions arise when the effective potential seen by the incident electron is capable of supporting one or more bound states. Feshbach resonances occur when the collisional complex forms a transient doubly excited state which subsequently decays by emission of an electron and the resonance lies energetically below the parent target state. Shape resonances occur when the intermediate state formed during the collision lies energetically above the parent target state, the electron is trapped by the centrifugal barrier and escapes by tunneling. The study of the effects of Coulomb interaction screening on the dynamic behavior of resonances when the screening strength changes is of significant interest and can provide an insight in the overall excitation dynamics.

The most prominent feature of the potential (1), which is the source of the new phenomena in the cross section behavior in the resonant region, is the lifting of the Coulomb l degeneracy of hydrogenic energy levels (see, e.g., [12]). The hydrogenic n threshold is now split into n components, the energy difference between which in-

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creases with decreasing the screening length D. Another important feature of the potential (1) is that for any finite value of D, it supports only a finite number of bound nl states. This implies that with decreasing D, the binding energies of nl states decrease and the nl energy levels successively enter in the continuum at certain critical screening D_{nl}, obeying the relations $D_{n+1,l} > D_{nl}$ and $D_{n,l+1} > D_{nl}$. For the $1s$, $2s$, and $2p$ states, the D_{nl} values are 0.840, 3.223, and 4.541 atomic units, respectively [13]. Furthermore, with decreasing D, the excitation threshold energies also decrease. For a given n, the states with lower l value have lower thresholds for any fixed value of D. As a consequence of the decrease of energies of bound states when D decreases, the corresponding wave functions become increasingly more diffuse, with obvious effects on the near-threshold processes.

The R-matrix method for electron-atom and photon-atom interactions has been discussed in detail by Burke *et al.* [14,15], and it is not necessary to repeat its description here. The physical orbitals of the hydrogen atom with the screened Coulomb potential (1) are calculated by piecewise exact power series expansions of the radial function [16], while the pseudo-orbitals are optimized by the CIV3 computer code [17]. The R-matrix code uses a modified version based on the UK [18,19] atomic R-matrix packages in which the Coulomb interactions in the $(N+1)$-electron nonrelativistic Hamiltonian are replaced by Yukawa-type screened Coulomb interactions (in atomic units):

$$H^{N+1} = \sum_{n=1}^{N+1}\left[-\frac{1}{2}\nabla_n^2 - \frac{Z}{r_n} * \exp(-r_n \cdot D^{-1}) + \sum_{m>n}^{N+1}\frac{1}{r_{mn}} * \exp(-r_{mn}\cdot D^{-1})\right], \tag{2}$$

where $\mathbf{r}_n$ is the electron radius vector (with respect to the nucleus Z), $r_{mn} = |\mathbf{r}_m - \mathbf{r}_n|$ is the interelectron distance, and D is the screening length. The electron-electron interaction term is expanded as [20,21]:

$$V_{\rm ee} = \frac{\exp(-r_{mn}D^{-1})}{r_{mn}} = \begin{cases} \sum_{l=0}^{\infty}\frac{r_<^l}{r_>^{l+1}}P_l(\cos\theta) & D^{-1}=0 \\ -D^{-1}\sum_{l=0}^{\infty}(2l+1)j_l(iD^{-1}r_<)h_l^{(1)}(iD^{-1}r_>)P_l(\cos\theta) & D^{-1}>0 \end{cases}, \tag{3}$$

where $r_> = \max(r_m, r_n)$, $r_< = \min(r_m, r_n)$, P_l, j_l, and $h_l^{(1)}$ are the Legendre polynomials, the spherical Bessel functions, and the spherical Hankel functions of the first kind with complex argument, respectively.

In order to check the sufficiency of the basis set used in our RMPS calculations, we have first considered the nonscreened case by using 14 physical states ($1s$-$5s$, $2p$-$5p$, $3d$-$5d$, $4f$, $5f$) and four pseudostates ($6s$, $6p$, $6d$, $6f$) in the expansion (2) and have calculated the $1s \rightarrow 2s$ and $1s \rightarrow 2p$ excitation cross sections and resonance parameters for the collision energy range between the $n=2$ and $n=3$ excitation thresholds. The latter were calculated by the eigenphase sum method [11,22]. Our results agreed very well with the 18-state basis variational results of Callaway [22] (up to four or five digits in the resonance parameters values), the benchmark cross section calculations of Bartschat *et al.* [23] (using the convergent close-coupling, RMPS, and intermediate-energy R-matrix methods), and the experimental data of Williams [24]. This test served as a guide to determining the size of the basis in the calculations with interaction screening. By checking the convergence of the results for each value of D, it was found that for $D < 30$ a.u., the accuracy of the results is not compromised if the number of physical states in the basis is progressively reduced (with decreasing of D) and the number of pseudostates is progressively augmented. This is a reflection of the fact that with decreasing D, the discrete states in the potential (1) successively enter in the continuum.

The most pronounced resonances in the $n=2$ threshold region in the nonscreened case are the ${}^1S^e(1,2,3)$, ${}^3S^e$, ${}^1P^o(1)$, ${}^3P^o(1,2)$, ${}^1D^e$ Feshbach resonances and the ${}^1P^o(2)$ shape resonance, and these have been thoroughly studied in the past. (The resonance with a given symmetry having a larger number in the parentheses is closer to the threshold.) Figure 1 shows the change of the width of resonances when D decreases from $D=\infty$ to $D=3.8$ a.u. The figure shows that with decreasing D, the width of a Feshbach resonance changes dramatically when it approaches the $2s$ threshold. The character of these changes is quite different for ${}^{1,3}S$ and for ${}^{1,3}P$, ${}^1D$ resonance. The widths of the

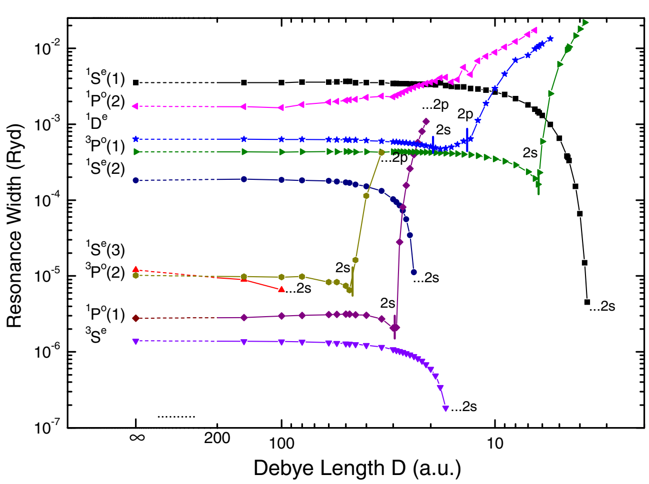

FIG. 1 (color online). The variation of the width of Feshbach and shape resonances when the screening length decreases. Short dashed lines represent the critical values of D where Feshbach resonances pass across the $2s$ or $2p$ threshold.

former, converging to the $2s$ threshold, rapidly decrease when the resonance approaches the threshold before it merges with the parent $2s$ state. [Note that for ${}^3S^e(3)$, this happens already at $D \sim 100 - 80$ a.u.] The widths of ${}^{1,3}P$ Feshbach resonances also considerably decrease when they approach the $2s$ threshold, but after passing it, their widths start to increase rapidly, a signature of the shape resonance [see the D dependence of the ${}^1P^o(2)$ shape resonance in Fig. 1]. The transformation of a ${}^{1,3}P$ Feshbach resonance into a shape resonance can be understood by taking into account the quasidegeneracy of $2s$ and $2p$ thresholds (even for finite D) in which case the two-electron states are described as $2snp \pm 2pns$ superpositions [25]. As demonstrated in [26] for ${}^1P$ states for the unscreened case, in the hyperspherical coordinate description of two-electron states the potential for the "$-$" state, defined above, supports bound states below the $n = 2$ threshold [corresponding to the ${}^1P^o(1)$ Feshbach resonance], while that for the "$+$" state it is not strong enough to support bound states but exhibits a potential barrier above the threshold which supports a quasibound state [corresponding to the ${}^1P^o(2)$ shape resonance]. In the screened case, because with decreasing D the wave functions become more and more diffuse, the $2p$ state can also mix with higher l states. Having in mind that for finite D the $2s$ and $2p$ thresholds are separated, this mixing produces a barrier in the "$-$" potential. Therefore, after passing the $2s$ threshold, the ${}^1P^o(1)$ state is prone to under-barrier decay (i.e., becomes a shape resonance). The same mixing, however, does not considerably change the existing barrier in the "$+$" potential. The mixing of the $2p$ state with the d states is also responsible for the change of character of the ${}^3P^o(1, 2)$ resonances. For the ${}^1P^o(1)$, ${}^3P^o(1)$, and ${}^3P^o(2)$ resonances, the critical screening length, D_c, where the Feshbach resonance passes the $2s$ threshold, lies in the regions 30–29 a.u., 48–45 a.u., and 6.3–6.2 a.u., respectively. We note that with decreasing D, the $2s$ threshold decreases, the wave functions of both bound and quasibound states become increasingly more diffuse, and both of these factors contribute to the rapid increase of the widths of shape resonances with decreasing D, as observed in Fig. 1.

The ${}^1D$ resonance in Fig. 1 shows specific behavior in the region of D between the $2s$ and $2p$ thresholds (19 a.u. $\geq D \geq$ 14 a.u.). The "$+$" and "$-$" superpositions for the ${}^1D$ resonance are made up of the $2snd$ and $2pnp$ two-electron states. The behavior of the width before and after passing the $2p$ threshold can be taken as an indication of the existence of two barriers in the system of "$\pm$" potentials. This behavior also suggests that only one of these potentials can support bound states. After passing the $2p$ threshold at $D_c \approx 13$ a.u., ${}^1D$ becomes a typical shape resonance with sharply increasing width.

It should be noted that the widths of shape resonances ${}^1P^o(2)$, ${}^3P^o(1)$, and ${}^1D^e$ become very large (larger than 0.015 Ry) for $D \leq 7$ a.u. $D \leq 4.2$ a.u., and $D \leq 5.0$ a.u., respectively, which makes their determination (as well as the resonance positions) rather uncertain. It is interesting to note that the ${}^3P^o(1)$ shape resonance survives down to 3.8 a.u. (the last D value of our investigations), despite the fact that the $2p$ state for $D < D_{2p} = 4.541$ a.u. is already in the continuum.

In Fig. 2, the $1s \rightarrow 2s$ [panels (a) and (b)] and $1s \rightarrow 2p$ [panel (c)] excitation collision strengths are shown in the

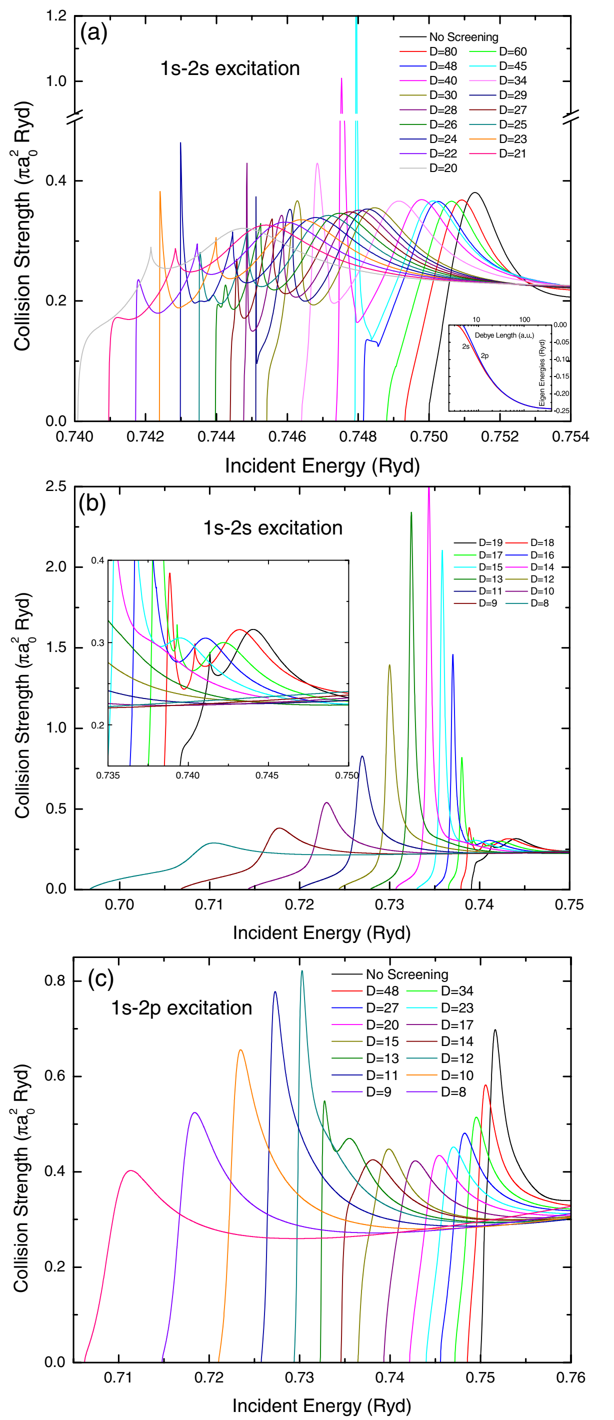

FIG. 2 (color online). Dynamic evolution of $1s \rightarrow 2s$ [panels (a) and (b)] and $1s \rightarrow 2p$ [panel (c)] collision strengths when the screening length varies (Debye length increases from left to right).

$n = 2$ resonant energy region when the screening length D decreases from $D = \infty$ to $D = 8$ a.u., and the binding energies of $2s$ and $2p$ states with changing D are shown in the inset in Fig. 2(a). The significant changes in the structure and values of the collisions strengths, especially for the $1s \rightarrow 2s$ transition, are obviously related to the changes of the resonance parameters when D decreases, particularly in the regions of D where ${}^{1,3}P$ and ${}^{1}D$ Feshbach resonances change their character. These peaks are clearly observed in the $1s \rightarrow 2s$ collision strength for $D = 45$ a.u. (at $E = 0.747\,94$ Ry) and for $D = 29$ a.u. (at $E = 0.745\,118$ Ry) in Fig. 2(a), where the ${}^{3}P^{o}(2)$ and ${}^{1}P^{o}(1)$ resonances have already acquired a shape-type character. The resonant structure in Fig. 2(b) reflects the effects of ${}^{1}D^{e}$ resonance on the $1s \rightarrow 2s$ collision strength after passing the $2s$ threshold at $D \approx 19$ a.u.. After passing the $2p$ threshold at $E = 0.739\,402$ Ry ($D = 13$ a.u.), the ${}^{1}D^{e}$ resonance gives the main contribution to the $1s \rightarrow 2p$ collision strength as seen in Fig. 2(c). [For $D > 14$ a.u., this collision strength in the energy range considered is dominated by the ${}^{1}P^{o}(2)$ shape resonance.]

The relatively small but sharp peaks (cusps) observed in the $1s \rightarrow 2s$ collision strength [see Fig. 2(a) and the inset of Fig. 2(b)] represent the effects of virtual states [27] associated with the ${}^{3}P^{o}(2)$ (for $D < 34$ a.u.), ${}^{1}P^{o}(1)$ (for $D < 21$ a.u.), and ${}^{1}S^{e}(2)$ (for $D < 27$ a.u.) when these states approach the $2p$ and $2s$ thresholds, respectively. We should note that similar virtual state effects have also been observed in the electron-helium excitation cross sections in the $n = 2$ thresholds region [27–29], where the Coulomb degeneracy is also lifted.

In conclusion, the present study has revealed that the screening of the Coulomb interaction has important effects on the electron-hydrogen atom excitation processes in $n = 2$ threshold region. The lifting of the Coulomb l degeneracy by the potential screening results in separation of $2s$ and $2p$ thresholds, which profoundly affects the dynamics of near-threshold excitation processes. It was found that the decrease of the screening length, D, leads to transition of Feshbach ${}^{1,3}P$ and ${}^{1}D$ resonances to shape-type resonances when D passes the critical value D_c for which the resonance position is equal to the corresponding threshold. This transition produces significant changes in the resonance width and, consequently, in the evolution of collision strength when D varies. Another important effect of the Coulomb interaction screening is the reduction of the number of resonances (as a result of the merging of ${}^{1,3}S$ resonances with their parent states and the rapid decay of shape resonances for small D). Although the present study was restricted to the $n = 2$ threshold energy range, the above conclusions have a general character. This has been confirmed by our RMPS calculations and resonance analysis in the energy range around the $n = 3$ thresholds. A detailed presentation of the evolution of collision strengths and resonance parameters for the $n = 2$ and $n = 3$ resonant regions when the screening length varies will be given in forthcoming papers.

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[1] D. Salzman, *Atomic Physics in Hot Plasmas* (Oxford University Press, Oxford, 1998).
[2] M. S. Murillo and J. C. Weisheit, Phys. Rep. **302**, 1 (1998).
[3] J. P. Hansen and I. R. McDonald, *Theory of Simple Fluids* (Academic, London, 1986).
[4] *Spectral Line Shapes*, edited by F. Rostas (Walter de Gruyter, New York, 1985), Vol. 3.
[5] A. V. Vinogradov and V. P. Shevelko, Sov. Phys. JETP **44**, 542 (1976).
[6] B. L. Whitten, N. F. Lane, and J. C. Weisheit, Phys. Rev. A **29**, 945 (1984); **30**, 650 (1984).
[7] J. K. Yuan, Y. S. Sun, and S. T. Zheng, J. Phys. B **29**, 153 (1996).
[8] Y.-D. Jung, Phys. Plasmas **2**, 332 (1995); **2**, 1775 (1995); **4**, 21 (1997).
[9] Y. Y. Qi, Y. Wu, J. G. Wang, and Y. Z. Qu, Phys. Plasmas **16**, 023502 (2009).
[10] Y.-D. Jung and J.-S. Yoon, J. Phys. B **29**, 3549 (1996).
[11] P. G. Burke and C. J. Joachain, *Theory of Electron-Atom Collisions* (Plenum, New York, 1995).
[12] L. D. Landau and E. M. Lifshitz, *Quantum Mechanics: Non-Relativistic Theory* (Pergamon, London, 1958).
[13] F. J. Rogers, H. C. Graboske, and D. J. Harwood, Phys. Rev. A **1**, 1577 (1970).
[14] P. G. Burke, A. Hibbert, and W. D. Robb, J. Phys. B **4**, 153 (1971).
[15] P. G. Burke, C. J. Noble, and V. M. Burke, Adv. At. Mol. Opt. Phys. **54**, 237 (2007).
[16] F. Salvat, J. M. Fernfindez-Varea, and W. Williamson, Jr., Comput. Phys. Commun. **90**, 151 (1995).
[17] A. Hibbert, Comput. Phys. Commun. **9**, 141 (1975).
[18] K. A. Berrington, W. B. Eissner, and P. H. Norrington, Comput. Phys. Commun. **92**, 290 (1995).
[19] Modified version of RMATRX-I, http://amdpp.phys.strath.ac.uk/rmatrix/.
[20] C. J. Joachain, *Quantum Collision Theory* (North-Holland Publishing Company, Amsterdam, 1975), p. 670.
[21] E. N. Economou, *Green's Functions in Quantum Physics* (Springer, Berlin, 2005), 3rd ed., p. 402.
[22] J. Callaway, Phys. Rev. A **26**, 199 (1982).
[23] K. Bartschat, I. Bray, P. G. Burke, and M. P. Scott, J. Phys. B **29**, 5493 (1996).
[24] J. F. Williams, J. Phys. B **21**, 2107 (1988).
[25] J. W. Cooper, U. Fano, and F. Prats, Phys. Rev. Lett. **10**, 518 (1963).
[26] C. D. Lin, Phys. Rev. Lett. **35**, 1150 (1975).
[27] P. G. Burke, J. W. Cooper, and S. Ormonde, Phys. Rev. **183**, 245 (1969).
[28] K. A. Berrington, P. G. Burke, and A. L. Sinfailam, J. Phys. B **8**, 1459 (1975).
[29] E. T. Hudson, K. Bartschat, M. P. Scott, P. G. Burke, and V. M. Burke, J. Phys. B **29**, 5513 (1996).