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# Widths of the doubly excited resonances of two-electron atoms below the $n = 2$ threshold

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We present an alternative theoretical procedure for the positions and widths of the doubly excited resonances of a two-electron atom based on a configuration-interaction procedure for *continuum* by using a $B$-spline-based finite basis set. More specifically, by examining the energy variation of the probability density corresponding to the singly excited ionization channel, the resonant energy $E_r$ of the doubly excited autoionization state can be directly linked to the energy at the minimum probability density. The width of the resonance can be identified with the energy separation between two energies, which are located on the opposite side of the center of the resonance and each corresponds to a probability density twice the minimum value at $E_r$. The effectiveness of this procedure is demonstrated by the excellent agreement between our calculated widths of the Feshbach resonance for $H^-$ and He below the $n = 2$ threshold and the ones from the most accurate existing theoretical calculations.

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The accuracy of an experimental determination of the resonant width $\Gamma$, which measures the interaction strength between the bound and continuum components of the state wave function of a doubly excited autoionization state, is often limited by the difficulty in unraveling the asymmetric structure profile, resulting usually from the simultaneous change of electronic orbitals of two electrons in a double-excitation process. For a narrow resonance, the width measurement could also be hampered by the lack of adequate energy resolution. As a result, for a two-electron atom, resonant widths are in general more readily available from the theoretical calculations than from the experimental measurements. Among the most accurate theoretical widths are the ones calculated by using the complex-coordinate rotational method [1,2], the pseudostate close-coupling method [3,4], the $R$-matrix theory [5,6], the $L^2$-basis method [7,8], the Feshbach projection method [9], and the Kuhn-Feshbach variation method [10]. Other theoretical calculations include the ones from the truncated-diagonalization method (TDM) [11], the simplified saddle-point technique [12], and the hyperspherical-coordinate method [13]. Except for the complex-coordinate rotational method, in which the width is given by the imaginary part of the energy eigenvalue, the resonant width is usually determined either by the energy variation of the calculated scattering phase shifts, or by the golden-rule formula, involving the interaction matrix between the bound and continuum components of the state wave function.

Following the recently proposed simple configuration-interaction procedure for *continuum* (CIC) with discretized $B$-spline-based finite basis set [14], the widths of the doubly excited autoionization resonances can also be derived, similar to other theoretical approaches, from the energy variation of the calculated scattering phase shifts. It is the purpose of this paper to point out that an alternative approach, also based on this simple CIC procedure, could potentially be more effective in the quantitative determination of the resonant width. In this approach, the resonant width is expressed in terms of its FWHM (i.e., full width at half maximum), corresponding to the cross sections for photoionization leading to the doubly excited resonance.

We start with the multiconfiguration state wave function $\Phi_E^\Lambda$ calculated from the simple CI procedure [14,15] for a state $|E\rangle$ corresponding to a total energy $E$, and a symmetry defined by a set of quantum numbers $\Lambda \equiv \{S, L, M_S, M_L\}$, i.e.,

$$\Phi_E^\Lambda = \sum_{\mu l l'} \Xi_{E,\mu l l'}^\Lambda , \tag{1}$$

where the configuration series function (or the *channel function*)

$$\Xi_{E,\mu l l'}^\Lambda = \sum_\nu C_E^\Lambda(\mu l, \nu l') \psi_{\mu l \nu l'}^\Lambda \tag{2}$$

represents the contribution to $\Phi_E^\Lambda$ from the $\mu l l'$ configuration series. The $\mu l l'$ series consists of a set of $LS$-coupled two-electron configuration functions $\psi_{\mu l \nu l'}^\Lambda$, with the inner electron occupying a fixed hydrogenic orbital $\mu l$, and the orbitals of the other $l'$ electron extended from negative to positive energy over a nearly complete set of hydrogenic functions. The probability density $\rho_{\mu l l'}$ for the configuration series $\mu l l'$ is defined in terms of its corresponding CI coefficients, i.e.,

$$\rho_{\mu l l'}(E) = \sum_\nu |C_E^\Lambda(\mu l, \nu l')|^2 . \tag{3}$$

At energy below the second ionization threshold, the continuum spectrum is dominated by a series of doubly excited resonances embedded in the $1sl$ open channel. The state wave function can be expressed as the sum of a single open-channel function $\Xi_{E,1sl}^\Lambda$ and a combined contribution that represents all doubly excited closed channels, i.e.,

$$\Phi_E^\Lambda = \Xi_{E,1sl}^\Lambda + \sum_{\mu_0 l_0 l'} \Xi_{E,\mu_0 l_0 l'}^\Lambda . \tag{4}$$

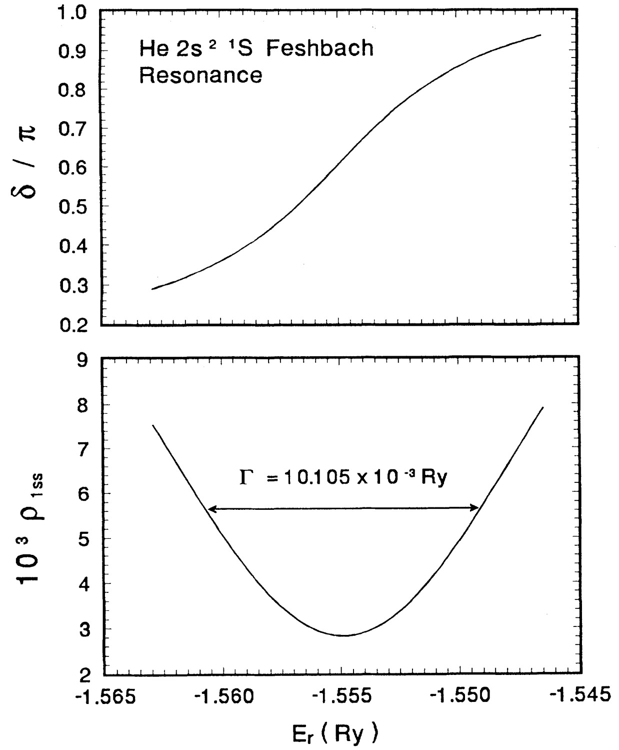

FIG. 1. Scattering phase shifts δ and the probability density $\rho_{1ss}$ of the 1*ss* ionization channel as functions of energy $E$ near the lowest He $^1S$ Feshbach resonance from a *zeroth order* CIC calculation, which includes the 1*ss*, 2*ss*, 2*pp*, 3*ss*, 3*pp*, and 3*dd* configuration series only.

As shown in Ref. [14], the open-channel function $\Xi^{\Lambda}_{E,1sl}$ can also be expressed in the form of $\psi^{\Lambda}_{1s\xi_{\varepsilon l}}$, where one of the orbital functions in $\psi^{\Lambda}$ is replaced by the radial function

$$\xi_{\varepsilon l}(r)=\sum_{\nu} C_E^{\Lambda}(1s,\nu l)\chi_{\nu l}(r) \ , \tag{5}$$

where ε is the kinetic energy of the ionized electron.

Physically, at the resonant energy $E_r$ of the doubly excited resonance, the contribution to $\Phi_E^{\Lambda}$ from all closed channels should be at its maximum and, as a result, $E_r$ can be linked directly to the energy at which the probability density $\rho_{1sl}$ of the ionization channel 1*sl* is at its *minimum* value. The probability density $\rho_{1sl}$ is also related to the energy-dependent amplitude $A$ of $\xi_{\varepsilon l}(r)$ at larger $r$, which is defined by Eq. (11) of Ref. [14], by

$$\rho_{1sl}(E)=\langle \xi_{\varepsilon l}(r)|\xi_{\varepsilon l}(r)\rangle \approx \frac{R}{2}A^2 \ , \tag{6}$$

where $R$ is the radius of the sphere that defines the $B$-spline-based finite basis set. The total energy $E$, or the outgoing electron energy ε, varies as we change the radius $R$ slightly in the CIC calculation. Since $R$ is approximately a constant and is also substantially greater than the $R$ variation $\Delta R$ required to cover the resonance, $\rho_{1sl}(E)$ is approximately proportional to $A^2$. In addition, it has already been shown in Ref. [14] that the photoionization cross section $\sigma$ in the CIC procedure is inversely proportional to $A^2$ [see Eq. (20) of Ref. [14]]. Consequently, $\sigma$ is inversely proportional to $\rho_{1sl}(E)$ for transitions leading to the doubly excited resonance with a nearly symmetric structure profile. As the probability density $\rho_{1sl}(E)$ approaches its minimum value at $E_r$, $\sigma \rightarrow \sigma_{\max}$, and as $E$ moves away from $E_r$, the cross section $\sigma$ decreases. Eventually, $\sigma$ is reduced to half of $\sigma_{\max}$ when $\rho_{1sl}(E)$ is doubled at $E_r \pm \Gamma/2$, where $\Gamma$ is the full width at half minimum. As a result, the positions and the widths of an entire series of doubly excited resonances can be estimated from the energy variation of the probability density of the ionization channel in a single CIC calculation.

In Fig. 1, we present the energy variation of $\rho_{1sl}$ for the lowest He $^1S$ Feshbach resonance below the $n=2$ threshold. A total of six configuration series, i.e., 1*ss*, 2*ss*, 3*ss*, 2*pp*, 3*pp*, and 3*dd*, are included in this *zeroth-order* CIC calculation. The nearly complete but finite set of hydrogenic orbital functions is expanded in terms of a set of $B$-spline polynomials [14,16,17], with its order $k=13$ and number $N$ ranging from 142 to 122 for the $s$, $p$, and $d$ orbitals. The radius $R$ is varied at values close to $120a_0$. The energy variation of the calculated scattering phase

TABLE I. Changes in width ($\Delta\Gamma$) (in rydbergs) due to the additional configuration series for the He $2s^2\,{}^1S$ and H$^-$ $sp2^+\,{}^3P$ Feshbach resonances.

| State | Configuration series | ΔΓ (Ry) | Γ (Ry) |
|---|---|---|---|
| He $2s^2\,{}^1S$ | *A* (1*ss*, 2*ss*, 2*pp*, 3*ss*, 3*pp*, and 3*dd*) | | $10.105\times10^{-3}$ |
| | *B* (*A* + all other *pp* series) | $-0.296\times10^{-3}$ | $9.809\times10^{-3}$ |
| | *C* (*B* + all other *ss* series) | $-0.471\times10^{-3}$ | $9.338\times10^{-3}$ |
| | *D* (*C* + all other *dd* series) | $-0.230\times10^{-3}$ | $9.108\times10^{-3}$ |
| | *E* (*D* + all *ff* and *gg* series) | $0.056\times10^{-3}$ | $9.164\times10^{-3}$ |
| H$^-$ $sp2^+\,{}^3P$ | *A* (1*sp*, 2*sp*, 2*ps*, 2*pd*, 3*sp*, 3*ps*, 3*pd*, 3*dp*, and 3*df*) | | $5.406\times10^{-4}$ |
| | *B* (*A* + all other *pd* series) | $-0.574\times10^{-4}$ | $4.832\times10^{-4}$ |
| | *C* (*B* + all other *df* series) | $-0.011\times10^{-4}$ | $4.821\times10^{-4}$ |
| | *D* (*C* + all other *sp* series) | $-0.574\times10^{-4}$ | $4.247\times10^{-4}$ |
| | *E* (*D* + all *fg* series) | $-0.002\times10^{-4}$ | $4.245\times10^{-4}$ |

TABLE II. Resonant energy $E_r$ (upper entry in rydbergs) and width $\Gamma$ (lower entry in $a[-b]=a\times10^{-b}$ Ry) for the Feshbach resonances of $H^-$ below the $n=2$ threshold.

| State | Present | $A$[a] | $B$[b] | $C$[c] | $D$[d] | $E$[e] |
|---|---|---|---|---|---|---|
| $^1S(1)$ | −0.297 546 | −0.297 566 | −0.297 553 |  |  | −0.297 580 |
|  | 3.54[−3] | 3.46[−3] | 3.462[−3] |  |  | 3.82[−3] |
| $^1S(2)$ | −0.252 035 |  | −0.252 042 |  | −0.252 034 | −0.252 012 |
|  | 1.83[−4] |  | 1.76[−4] |  | 1.82[−4] | 1.91[−4] |
| $^3S$ | −0.254 208 |  | −0.254 208 |  |  | −0.254 216 |
|  | 1.34[−6] |  | 1.34[−6] |  |  |  |
| $^1P$ | −0.252 098 |  | −0.252 099 6 | −0.251 945 | −0.252 099 2 | −0.252 085 |
|  | 2.94[−6] |  | 2.64[−6] | 2.10[−6] | 2.73[−6] |  |
| $^3P(1)$ | −0.284 299 | −0.284 262 | −0.284 273 | −0.284 232 |  | −0.284 057 |
|  | 4.25[−4] | 4.28[−4] | 4.26[−4] | 4.37[−4] |  | 5.22[−4] |
| $^3P(2)$ | −0.250 789 |  | −0.250 820 | −0.250 705 |  |  |
|  | 1.39[−5] |  | 9.47[−6] | 1.08[−5] |  |  |
| $^1D$ | −0.255 855 | −0.255 811 | −0.255 874 |  |  | −0.255 760 |
|  | 6.34[−4] | 6.48[−4] | 6.33[−4] |  |  | 6.47[−4] |

[a] Scholz, Scott and Burke [5].
[b] Ho, and Bhatia and Ho [1].
[c] Ajmera and Chung [10].
[d] Callaway [4].
[e] Pathak, Kingston, and Berrington [6].

TABLE III. Resonant energy $E_r$ (upper entry in rydbergs) and width $\Gamma$ (lower entry in $a[-b]=a\times10^{-b}$ Ry) for selected Feshbach resonances of He below the $n=2$ threshold.

| State | Present | $A$[a] | $B$[b] | $C$[c] | $D$[d] | $E$[e] |
|---|---|---|---|---|---|---|
| $2s2s\ ^1S$ | −1.555 71 | −1.5556 | −1.555 736 | −1.555 76 |  | −1.556 82 |
|  | 9.16[−3] | 9.16[−3] | 9.06[−3] | 6.67[−3] |  | 9.04[−3] |
| $2s3s\ ^1S$ | −1.179 77 | −1.179 73 | −1.179 79 | −1.179 91 |  | −1.179 85 |
|  | 2.73[−3] | 2.76[−3] | 2.70[−3] | 1.85[−3] |  | 2.68[−3] |
| $2p2p\ ^1S$ | −1.243 108 | −1.243 032 | −1.243 855 | −1.244 51 |  | −1.238 554 |
|  | 4.42[−4] | 4.62[−4] | 4.31[−4] | 1.29[−3] |  | 5.72[−4] |
| $2s3s\ ^3S$ | −1.205 155 | −1.205 153 5 |  |  |  |  |
|  | 1.33[−5] | 1.284[−5] |  |  |  |  |
| $2p3p\ ^3S$ | −1.119 484 | −1.119 437 4 |  |  |  |  |
|  | 4.8[−7] | 4.6[−7] |  |  |  |  |
| $sp2^+\ ^1P$ | −1.386 103 | −1.3856 | −1.386 27 | −1.385 50 | −1.385 65 | −1.384 26 |
|  | 2.78[−3] | 2.66[−3] | 2.75[−3] | 2.69[−3] | 2.68[−3] | 2.75[−3] |
| $sp3^+\ ^1P$ | −1.128 108 | −1.128 02 | −1.1280 | −1.127 674 | −1.128 18 | −1.127 58 |
|  | 6.08[−4] | 6.2[−4] | 6.02[−4] | 6.20[−4] | 5.84[−4] | 6.21[−4] |
| $sp3^-\ ^1P$ | −1.194 147 | −1.194 145 | −1.194 148 | −1.194 106 | −1.194 39 | −1.194 60 |
|  | 7.67[−6] | 7.78[−6] | 7.70[−6] | 6.95[−6] | 7.23[−6] | 1.05[−5] |
| $sp2^+\ ^3P$ | −1.520 949 | −1.520 902 | −1.520 985 | −1.521 712 | −1.521 224 |  |
|  | 5.80[−4] | 6.02[−4] | 5.94[−4] | 7.72[−4] | 6.01[−4] |  |
| $sp3^+\ ^3P$ | −1.169 334 | −1.169 304 | −1.169 345 | −1.169 524 | −1.169 437 |  |
|  | 1.58[−4] | 1.54[−4] | 1.65[−4] | 1.37[−4] | 1.68[−4] |  |
| $sp3^-\ ^3P$ | −1.158 055 | −1.158 049 | −1.158 062 | −1.157 992 | −1.158 330 |  |
|  | 3.95[−6] | 3.56[−6] | 3.78[−6] | 3.98[−6] | 4.12[−6] |  |

[a] Oza [3].
[b] Ho [1].
[c] Wu and Xi [12].
[d] Moccia and Spizzo [7].
[e] Macias and Riera [8].

shifts δ across the resonance is also shown, together with $\rho_{1sl}$, for comparison. As expected, the estimated width of $10.105\times10^{-3}$ Ry from the $\rho_{1sl}$ variation equals the width determined by a least-squares fit of the phase shifts.

To improve the accuracy of the resonant width, more configuration series, representing various $ll'$ combinations, are required in the CIC calculation. In particular, if the widths are to be determined from the energy variation of the phase shifts, the $B$-spline set typically requires a size of $N \geq 120$ for a four- to five-digit convergence in phase shifts. Computationally, this will lead to a prohibitively large total number of configurations in the CIC calculation. To reduce the size of the basis set, the present CIC calculation is carried out in two separate steps.

First, a *zeroth-order* CIC calculation, such as the one leading to the results presented in Fig. 1, is performed by including only a limited number of dominating configuration series in a basis set, which is constructed from $B$-spline sets of $N$ greater than 120. In addition, we carry out a similar zeroth-order CIC calculation with the same configuration-series combination, which employs $B$-spline sets of significantly smaller $N$ ranging from 30 to 50. In our second step, a substantially larger number of configuration series of various allowed $ll'$ combinations is included in calculating $E_r$ and Γ from the energy variation of the probability density. We are able to limit the total number of configurations at a manageable level (i.e., approximately 3000) by using the $B$-spline sets with the *same* smaller $N$ employed in the zeroth-order calculation. The change in $E_r$ and Γ due to the additional configuration series is estimated by comparing the zeroth-order $E_r$ and Γ with the ones from the complete calculation, both using the same $B$-spline set of *smaller* $N$. By adding the change in $E_r$ and Γ to the zeroth-order results using $B$-spline sets of *larger* $N$, we finally obtain our best estimated values for $E_r$ and Γ. The changes in Γ for the lowest He $^1S$ resonance and the lowest $H^-$ $^3P$ resonance, due to the addition of various $ll'$ configuration series, are illustrated in Table I. Table II presents our calculated $E_r$ and Γ for the Feshbach resonances of $H^-$ below the $n=2$ threshold. The agreement between the present results and those from a few selected calculations is excellent. Similar excellent agreement is also shown in Table III for a few selected Feshbach resonances of He. The maximum estimated uncertainty, in terms of the momentum $k$ of the ionized electron, is approximately $\pi/kR$, which is about 5% and 2% for $H^-$ and He, respectively. More extensive tabulation of $E_r$ and Γ will be presented elsewhere.

One of the most important advantages of the present theoretical procedure is its ability for immediate extension to atoms beyond two-electron systems. In fact, the $B$-spline based CI procedure has already been applied extensively to other two-electron and divalent atoms, such as the alkaline-earth atoms and their corresponding isoelectronic sequences [14,18,19]. The present procedure should further facilitate its application to the theoretical estimation of the positions and widths of the highly correlated doubly excited resonances in complex atoms.

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