

Double Rydberg formula and applications to doubly excited states of highly charged ions

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The screening constant in the double Rydberg formula is estimated using the intrashell configuration-interaction states. Its explicit dependence on the bending rovibrational quantum numbers is included. Comparison of the energy levels so obtained with elaborate numerical results indicates its utility for doubly excited states of highly charged ions and also points to its geometrical origin. Procedures are introduced to generalize the formula to intershell doubly excited states and to doubly excited states of multielectron atoms. A number of specific numerical results are presented.

I. INTRODUCTION

The identification and classification of doubly excited states¹ has been one of the central themes of theoretical and experimental investigations in recent years. For neutral atoms these states have been observed by single-photon or multiphoton absorption.^{2,3} For negative ions these states have been identified by measuring the yield of metastable atoms resulting from electron-impact excitations.⁴ In these experiments doubly excited states are formed through electron-electron correlations. In recent years doubly excited states of positive ions have been observed in the collisions of multiply charged ions with atoms by translational spectroscopy⁵ or by zero-degree spectroscopy.⁶ In these collisions doubly excited states are formed most frequently by double-electron-capture processes⁷ or by simultaneous electron capture and excitation of the projectiles.

Despite intensive studies over the years, our knowledge of doubly excited states is still limited. Experimental identification of individual doubly excited states is hampered by the need of high-resolution electron or ion spectroscopy. Theoretical studies are handicapped by the slow convergence of computational approaches and by the need of dealing with many doubly excited states in a narrow energy region. Extensive calculations have been completed only for some low-lying doubly excited states of helium and several low- Z heliumlike ions. Even today the energy levels of doubly excited states remain thus largely unknown.

In this paper we present a simple approximate formula known as the double Rydberg formula⁸ for estimating the energy levels of a certain class of doubly excited states of atoms. Our formula is based on the current understanding of the correlation of two excited electrons in the framework of the recently proposed classification scheme.⁹ Similar double Rydberg formulas were derived by Read⁸ and by Rau¹⁰ previously in connection with the energy levels of negative ions. Our derivation and interpretation differ from theirs.

This paper is organized as follows. Section II derives

the double Rydberg formula from the variational principle applied to intrashell configuration-interaction (CI) states of two-electron atoms and ions. The results depend on a screening constant which is given analytically in terms of correlation quantum numbers. This permits the estimate of energy positions of doubly excited states for two-electron atoms and ions without any fitting or empirical parameters. Section III examines the validity of the derived expression by comparison with elaborate numerical results. We discuss implications of this comparison and the relationship of our model with those of Read and Rau. Section IV outlines applications of the formula to estimating energy levels of intershell states, multielectron intrashell states, and predicting irregularities in decay width. Section V concludes the paper.

II. DERIVATION OF THE DOUBLE RYDBERG FORMULA FOR TWO-ELECTRON ATOMS

The double Rydberg formula is a compact representation of the energy levels of a particular type of atomic states in which a pair of electrons are located at about equal distances from the nucleus. In the case of two-electron atoms or ions presented here, the formula involves a mutual screening constant which pertains to the geometry of the two electrons. This constant can be derived in a simple variational manner using intrashell CI states. We rewrite the two-electron Hamiltonian as

$$H = \left[-\frac{1}{2} \nabla_1^2 - \frac{Z^*}{r_1} \right] + \left[-\frac{1}{2} \nabla_2^2 - \frac{Z^*}{r_2} \right] + (Z^* - Z) \left[\frac{1}{r_1} + \frac{1}{r_2} \right] + \frac{1}{r_{12}}, \quad (1)$$

where Z^* is an effective charge, and Z is the total charge of the nucleus. The wave functions are assumed to be a linear superposition of products of Coulomb wave functions corresponding to a screen charge Z^* . For intrashell states, we limit the superposition to products of hydrogenic wave functions with principal quantum number N , then

$$\left\langle \frac{1}{r_1} \right\rangle = \left\langle \frac{1}{r_2} \right\rangle = \left\langle \frac{1}{r} \right\rangle = \frac{Z^*}{N^2}. \quad (2)$$

In the CI approach, one would then evaluate the $1/r_{12}$ integral within the subspace and then diagonalize the total Hamiltonian. Here we take advantage of the fact that the two electrons, being at about equal distances away from the core, have the expectation value of $1/r_{12}$ which is proportional to $\langle 1/r \rangle$. By using the following approximation,

$$\langle 1/r_{12} \rangle = \left\langle \frac{1}{r} \right\rangle \frac{1}{(2 - 2\langle \cos\theta_{12} \rangle)^{1/2}} = \frac{Z^*}{N^2} (2\sigma), \quad (3)$$

where the proportionality constant 2σ is related to the geometry of the electron pair through the average value of $\cos\theta_{12}$. This approximation leads to the following expression for $\langle H \rangle$:

$$\sigma^{(1)} = \frac{2}{\left[24 + \frac{2}{N^2} [7(N+K-1)(N+K+1) + 7T^2 - 6L(L+1) + 12] \right]^{1/2}}. \quad (6)$$

In (6), K and T are angular correlation quantum numbers whose range is¹³

$$T = 0, 1, 2, \dots, \min(L, N-1), \quad (7)$$

$$K = (N-1-T), (N-3-T), \dots, -(N-1-T);$$

$T=0$ is not allowed if the parity of the state is $(-1)^{L+1}$.

Note how the correlation quantum numbers are exploited in the new classification scheme. A doubly excited state is denoted by ${}_n(K, T)_N^A 2S+1L^\pi$ where A indicates the type of radial correlation and is closely related to the spin and angular degrees of freedom,

$$A = \pi(-1)^{S+T}, \quad K > L - N$$

$$= 0, \quad K \leq L - N. \quad (8)$$

For intrashell states, $n=N$ and $A=+1$. Here N is the principal quantum number of the inner electron and n that of the outer electron.

Returning now to the screening constant, a less accurate but "simpler" expression for $\langle \cos\theta_{12} \rangle$ has also been derived by Herrick¹⁴ using $O(4)$ theory, namely

$$\langle \cos\theta_{12} \rangle = -\frac{3K}{2N}. \quad (9)$$

It is valid when K is positive and not differing too much from $N-1$. Equation (9) leads to

$$\sigma^{(2)} = \frac{1}{2(2+3K/N)^{1/2}}. \quad (10)$$

An alternative expression for σ can be derived using different approximations for $1/r_{12}$. Crance and Armstrong¹⁵ have given a group theoretical expression for r_{12}^2 and then they approximate $\langle 1/r_{12} \rangle$ by $1/(r_{12}^2)^{1/2}$. Using their result, one obtains, for example, for $1S^e$ states the result

$$\langle H \rangle = -\frac{Z^*}{N^2} (2Z - Z^* - 2\sigma). \quad (4)$$

Setting the variation of $\langle H \rangle$ with respect to Z^* equal to zero yields

$$\langle H \rangle = E_{N,N} = -\frac{(Z-\sigma)^2}{N^2} \quad (\text{a.u.}), \quad (5)$$

which expresses the energy of each doubly excited state in terms of a screening parameter σ . The screening parameter is related to the average of $\cos\theta_{12}$ for that state. Theoretical studies of doubly excited states have shown that the angular correlation as characterized by $\langle \cos\theta_{12} \rangle$, differs greatly for different states.¹¹ A convenient approximate expression for $\langle \cos\theta_{12} \rangle$ has been given by Herrick *et al.*¹² using the $SO(4)$ group theory from which

$$\sigma^{(3)} = \frac{1}{\left[5 + \frac{33}{4N^2} (N-K-1)^2 + \frac{19}{N^2} \right]^{1/2}}. \quad (11)$$

For ${}_N(N-1, 0)_N^+ 1S^e$ intrashell states, $\sigma^{(1)}$ and $\sigma^{(3)}$ approach 0.224 and 0.162, respectively, as N approaches infinity. These limiting values are smaller than the value 0.25 obtained by Read⁸ and Rau.¹⁰ The major difference is due to the fact that both Eqs. (6) and (11) were derived by including only intrashell states and assuming that the equality of r_1 and r_2 holds in the sense of average, while both Read and Rau obtain the results under the more strict condition that $r_1=r_2$.

III. VALIDITY OF THE FORMULA AND DISCUSSIONS

A basic assumption of the present model is that the two electrons are limited to the same average distance from the nucleus, i.e., the radial degrees of freedom are restricted. From the CI point of view, this is equivalent to assuming that all the hydrogenic orbitals used in the CI expansion has $n=N$. In an earlier analysis,¹⁶ it has been shown that the approximate wave functions obtained from the $SO(4)$ theory is adequate for states with $K > 0$, particularly for $K=N-1$ states. It fails for negative K since for $K < 0$, the two electrons are on the same side of the nucleus and they could maintain such an angular correlation pattern only by forcing $r_1 \neq r_2$ in order to minimize the Coulomb repulsion between them. Since intrashell states with negative K do not satisfy the assumptions used in the present derivation, it is not desirable to use Eq. (5) for $K < 0$ states.

To check the validity of the simple formula, we show in Table I energy levels of several selected intrashell doubly excited states for $N=3$ and 4. The states are designated using the new classification scheme. Each corresponds to the lowest state of the given N, L, S , and π . The energies

TABLE I. Comparison of energy levels of doubly excited states of heliumlike ions using the simple formula Eq. (5) with the results from the CI calculations by Bachau (Ref. 15) (shown in parentheses). All the energies are given in electron volts and are measured from the double ionization threshold. The screening σ was calculated using Eq. (10) for $^1S^e$ and $^1P^o$ and (6) for $^1D^e$.

Charge	Energies (eV)	
	$^3(2,0)_3^+ ^1S^e$	$^4(3,0)_4^+ ^1S^e$
Z = 5	68.21 (69.09)	38.48 (39.05)
6	99.90 (101.00)	56.37 (57.06)
7	137.75 (138.99)	77.56 (78.45)
8	181.59 (182.99)	102.34 (103.23)
9	231.47 (233.05)	130.43 (131.42)
10	287.41 (289.16)	161.91 (163.04)
	$^3(1,1)_3^+ ^1P^o$	$^4(2,1)_4^+ ^1P^o$
Z = 5	67.11 (67.48)	38.09 (38.47)
7	136.18 (136.62)	77.09 (77.60)
9	229.43 (229.92)	129.70 (130.34)
	$^3(2,0)_3^+ ^1D^e$	$^4(3,0)_4^+ ^1D^e$
Z = 5	67.72 (68.24)	37.95 (38.83)
7	137.05 (137.74)	76.89 (78.12)
9	230.56 (231.42)	129.43 (130.99)

calculated using (5) are compared with those calculated by Bachau¹⁷ using the CI method. Typically the difference is about 1 eV or less. This accuracy is adequate for the purpose of identifying the states observed in energy-gain spectroscopy. Note that our results are in principle (and in practice) inferior to those obtained by an intrashell CI calculation. The advantage is its ready availability for estimating energy levels when there are no theoretical calculations.

The relative error in applying Eq. (5) to doubly excited states of $Z=1$ and 2 atoms are larger. For the lowest $^1S^e$ states of H^- in the $N=4, 5$, and 6 manifolds, we compared (5) with the results of Ho¹⁸ and of Ho and Callaway.¹⁹ While the absolute errors are only 0.102, 0.070, and 0.048 eV for $N=4, 5$, and 6, respectively, the relative errors are about 9.5% in all three cases. These errors are inherent in the assumptions of SO(4) theory used in deducing $\langle \cos\theta_{12} \rangle$. Alternatively, we can evaluate the screening constant σ from Bachau's CI energy levels by inverting Eq. (5). We found that the so-determined numerical σ is almost constant along an isoelectronic sequence. For $^3(2,0)_3^+ ^1S^e$ and $^4(3,0)_4^+ ^1S^e$, the fitted σ are 0.219 and 0.207, respectively. These are to be compared with 0.250 and 0.243, respectively, obtained from Eq. (5). The insensitivity of σ to Z supports its geometrical origin. In principle, one can obtain a better estimate of energy levels by treating σ as a fitting parameter or introducing a quantum defect d to the denominator. This has to be done for each N, K , and T and it can be a subject of future study.

In the rest of this section, we discuss the relevance of the present model to the double Rydberg models of Read⁸ and Rau.¹⁰ Both authors invoke the arguments based on

the hyperspherical coordinates. In terms of the hyperradius R and the hyperangle α where $R=(r_1^2+r_2^2)^{1/2}$ and $\alpha=\arctan(r_2/r_1)$, the potential surface V can be expanded near the saddle point ($\alpha=45^\circ$ and $\theta_{12}=180^\circ$) as

$$V=Z_0/R-Z_c(\alpha-\pi/4)^2/R+Z_d(\theta_{12}-\pi)^2/R, \quad (12)$$

where $Z_0=2\sqrt{2}(Z-\frac{1}{4})$, and Z_c and Z_d are two other constants irrelevant to the present discussion. Read⁸ rewrites (12) as

$$-\frac{Z_0}{R}=-\frac{2\sqrt{2}(Z-\frac{1}{4})}{R}=-\frac{(Z-\frac{1}{4})}{r_1}-\frac{(Z-\frac{1}{4})}{r_2}, \quad (13)$$

upon using $r_1=r_2=R/\sqrt{2}$. Combining with the kinetic energy term of each electron, the local Hamiltonian is equivalent to the sum of two noninteracting electrons, each experiencing an effective charge $(Z-0.25)$. The intrashell energy levels are given by

$$E(N,N)=-\frac{(Z-\frac{1}{4})^2}{N^2} \quad (\text{a.u.}), \quad (14)$$

quite similar in form to Eq. (5). In fact they are identical for the state $^3(2,0)_3^+ ^1S^e$ for which σ is exactly 0.25.

Rau²⁰ took a somewhat different approach. By retaining only the first term of the potential in (12), he solved the Coulomb problem in the six-dimensional space. An energy expression similar to the Coulomb energy level with effective charge $Z-0.25$ was derived. To account for the fact that the potential away from the saddle point is not given by $-Z_0/R$, Rau introduced two additional parameters S_1 and S_2 to arrive at an empirical expression

$$E_v=-\frac{4(Z-\frac{1}{4}-S_1)^2}{(v+\frac{3}{2}-S_2)^2} \quad (\text{a.u.}), \quad (15)$$

for the energies of doubly excited states. The parameters S_1 and S_2 are obtained by fitting Eq. (15) to theoretical or experimental levels. An equation similar to (15) was also derived by Feagin and Macek²¹ by analyzing the asymptotic wave function of doubly excited states near the double-electron escape limit. They have an analytical expression for S_1 differing from Rau's empirical one.

We note that although the energy-level expression derived here is similar to those given by Read, Rau, Feagin and Macek, the underlying physical models are actually very different. Our derivation is an approximation to the intrashell CI calculation, thus the formula is expected to be more appropriate for low-energy states and for positive ions than for neutral atoms or negative ions. Though limited to such cases, our formula reveals specific dependence of σ on angular correlation quantum numbers K and T . Assessing the validity of other models lies outside the scope of this paper.

IV. FURTHER APPLICATIONS

A. Energy levels for intershell states of two-electron systems

Doubly excited states with the same L, S, π, K, T, A , and N belong to the same channel and n labels the states

of this channel. For neutral atoms and positive ions, n ranges from N to infinity if $A = +1$ and these states form a Rydberg series, the intrashell state $n = N$ being the first member. According to the Ritz-Rydberg formula, the energy levels for the whole series can be expressed as

$$E(n, N) = E_N - \frac{(Z-1)^2}{2(n-d)^2} \quad (\text{a.u.}), \quad (16)$$

where $E_N = -Z^2/2N^2$ is the N th hydrogenic energy level representing the channel's ionization limit and d is the usual quantum defect. Using the energy expression (5) for $E(N, N)$, the quantum defect for the whole series can be calculated by assuming that d is independent of n . We compare in Table II several energy levels of heliumlike boron calculated using this prescription with the CI results of Lipsky *et al.*²² They agree to within a few tenths of an eV. Note, however, that this prescription applies only to intershell states for which $A = +1$. Although the quantum defect is weakly energy dependent even for the series with $A = -1$ or 0, no simple extrapolation of d is possible because they do not have intrashell states. On the other hand, the $A = -1$ and $A = 0$ series are rarely produced in single-photon absorption² or in electron-impact excitation.²³ It is not known experimentally whether these states are produced efficiently in ion-atom collisions.

B. Doubly excited states of multielectron atoms

Doubly excited states of multielectron atoms consist of an electron pair outside a compact open-shell core. By defining the energy of the electron pair with respect to the open-shell core, the energy level of the pair can be generalized from Eq. (5) to

$$E_{N,N} = -\frac{(Z-\sigma)^2}{(N-\mu)^2} \quad (\text{a.u.}), \quad (17)$$

where μ is the quantum defect representing the penetration of an outer electron into the core region. Alternatively we can use μ as a fitting parameter⁸ in which case Eq. (17) can be interpreted as a semiempirical expression. To see the accuracy of such a fitting procedure, we examine the energy levels of He^- observed by Buckman *et al.*⁴ They denoted the observed doubly excited series as $1sN_s^{-2}S^e$ with $N = 3-8$. According to our notation, they should be designated as $1s_N(N-1, 0)_N^+ S^e$. Deducing the

TABLE II. Energy levels of some intershell states of heliumlike Boron ($Z = 5$) calculated using Eqs. (5) and (16) and the results are compared with those by Lipsky *et al.* (Ref. 22). Energies are measured in electron volts from the double ionization threshold.

State	Eqs. (5) and (16)	Ref. 22
$4(2, 0)_3^+ S^e$	53.91	54.19
$5(2, 0)_3^+ S^e$	47.76	47.96
$4(2, 0)_3^+ D^e$	53.72	53.72
$5(2, 0)_3^+ D^e$	47.66	47.72
$4(1, 1)_3^+ P^o$	53.50	53.17
$5(1, 1)_3^+ P^o$	47.57	47.39

quantum defect μ from Eq. (17) for the lowest state $N = 3$, we can evaluate the energy levels for other N 's and the results are compared with the measurement of Buckman *et al.*⁴ in Table III. (The reader should consult Ref. 8 for the determination of μ for doubly excited states outside a core whose energy is split by spin-orbit and spin-spin interactions.) The agreement between the measured values and those calculated from (17) is good.

The simple formula (17) allows us to organize the energy levels of doubly excited states along the isoelectronic sequence. We have already seen that the screening constant σ is independent of charge Z . The results shown in the previous paragraph indicate that μ is nearly independent of N . We expect that μ depends only weakly on Z and can be expressed as

$$\mu = \frac{a}{Z} + \frac{b}{Z^2} + \frac{c}{Z^3}, \quad (18)$$

where a , b , and c are treated as fitting parameters. Note that we treat σ to have the known dependence on K , T , and N as given by Eq. (6), while μ is expected to vary from one series to another and obtained from fitting. To check how well this procedure works, we first calculate the energy level of the $1s_3(2, 0)_3^+ S^e$ state for $Z = 10$ using the MCHF program of Froese-Fisher.²⁴ The calculated energy is then fitted to Eq. (17) to extract the quantum defect μ . From the calculated μ , we evaluate the binding energy of $1s_5(4, 0)_5^+ S^e$ state using (17). The result is -85.05 eV which is to be compared with -85.10 eV calculated from the MCHF program. We have also calculated the energies of $1s_3(2, 0)_3^+ S^e$ for $Z = 18$ and 36 to extract the quantum defects. These quantum defects for $Z = 10$, 18, and 36 are then fitted to Eq. (18) to obtain the following constants: $a = 0.4214$, $b = 0.08515$, and $c = 1.3085$. Using these constants, the energy levels of $1s_N(N-1, 0)_N^+ S^e$ for any Z can be calculated. We have tested this method for a few Z , and the results are quite satisfactory. Our main point here is to illustrate a method of organizing energy levels of doubly excited states along the isoelectronic sequence in the future. For example, one can generalize the method of organizing energy levels to

TABLE III. Energy levels of $\text{He}^{-2}S^e$ resonances measured from the two-electron ionization limit at $I = 24.588$ eV. Experimental energy of Buckman *et al.* (Ref. 4) for $N = 3$ is used to derive a quantum defect. Equation (16) is then used to calculate the energies for all the higher N states. The quotes around the $N = 8$ entry signify that Buckman *et al.* quote it only tentatively. Numbers in parentheses in the second column indicates the uncertainty in last digits. The energies are given in electron volts.

N	Experiment	Eq. (16)
3	2.138(5)	2.138
4	1.145(5)	1.154
5	0.728(5)	0.723
6	0.500(10)	0.493
7	0.372(10)	0.358
8	"0.282"	0.272

doubly excited states with the $1s^2 1S^e$, $1s^2 2s^2 S^e$, and $1s^2 2s^2 1S^e$ cores.

C. Irregularities in decay width

In general, the energy levels of a Rydberg series ${}_N(K, T)_N^{A 2S+1L^\pi}$ lie above the $(N-1)$ th ionization threshold. They autoionize predominantly²⁵ to the continuum channel with $N'=N-1$, and $K'=K-1$ with all the other quantum numbers fixed. From the energy of the N' th threshold, one can calculate the energy of the autoionized electron. One would like to know if the energy of the autoionized electron and its decay width follow some simple Z dependence for ready interpolation or extrapolation along the isoelectronic sequence.

This simple expectation fails since the energy level of the doubly excited state ${}_N(K, T)_N^{A 2S+1L^\pi}$ may lie below the $(N-1)$ th hydrogenic threshold, and energetically it can decay predominantly to the next lower threshold; the $(N-2)$ th threshold. This crossover occurs along the isoelectronic sequence, and when this happens the decay width becomes suddenly narrow and the autoionized electron has relatively large kinetic energy. Indeed we can find evidence of this sudden change in the calculation of Bachau¹⁷ already. Using Eq. (5) we find that for ${}_N(N-1, 0)_N^{+1S^e}$ states, the crossover occurs at $N=18$ for $Z=1$, at $N=5$ for $Z=2-4$, and at $N=4$ for $Z=5-20$. [The $N=18$ for $Z=1$ is definitely an overestimate. Using the empirical screening constant for H^- in Eq. (5) would predict that the crossover occurs at $N=10$.]

The above irregularity of decay widths along the isoelectronic sequence can also occur with increasing N for a given Z . Except for Bachau's, neither experimental nor theoretical information about such dependence is available so far because observations requires high resolution in energy.

V. CONCLUSION

In summary, we have shown that the approximate energy levels of doubly excited states can be calculated using a simple formula. It was derived on the basis of the new classification scheme of doubly excited states. For two-

electron atoms, there is no empirical parameter in the formula and the results are shown to be in reasonable agreement with *ab initio* calculations. The formula was derived for intrashell states under the assumption of strong angular correlations of the two electrons. They are equivalent to the results one would get in a limited approximate CI calculation. For the doubly excited states of multielectron atoms, we show that the energy levels can be organized by introducing a single quantum defect parameter which can be determined empirically or through *ab initio* calculation of a single state for each given double Rydberg series. We have also discussed how to estimate the energy levels of intershell states of a series if the first member of the series is an intrashell state. We conclude by noting that the formula presented here is for simple estimates of energy levels. More accurate results can be obtained by more sophisticated fitting procedure and/or *ab initio* calculations. Due to the irregularity, the calculations of decay width must be performed for each individual doubly excited state. The formula presented here is especially useful for estimating what doubly excited states are likely to be populated in the collision of multiply charged ions with atoms.

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