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Helium doubly excited states with zero angular momentum and electrons located on the same side of the nucleus

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A particular set of two-electron atomic resonances for the helium atom with zero total orbital angular momentum (S states) has been recently studied theoretically [K. Richter and D. Wintgen, J. Phys. B **24**, L565 (1991)]. These resonances essentially have both electrons on the same side of the nucleus and the outer electron "frozen." The present work suggests that the energies of these resonances correspond, when the degree of excitation of both electrons increases, to the energies of resonances associated with the Hamiltonian $H=p^2/2+p'^2/2-Z/r-Z/r'+1/||r|-|r'||$ in a space where both particles have zero angular momentum ($\ell=\ell'=0$). Moreover, the energy of each of these resonances appears to be that of the lowest member of an almost unperturbed Rydberg series of resonances converging to a single ionization threshold of He. The analysis of the problem relies on the method of o(4,2) operator replacements generalized by the method of complex scaling.

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I. INTRODUCTION

Classically stable planetary atomic configurations with zero total orbital angular momentum have been reported by Richter and Wintgen [1]. The electrons arrange themselves around a collinear periodic orbit with both localized on the same side of the nucleus. The outer electron is dynamically localized near some fixed radial distance [1]. A semiclassical treatment [1,2] suggests the energies E, associated with these resonances, form a Rydberg series converging to the three-particle breakup threshold, also called the double-ionization threshold:

$$E=-\{S/[j+\tfrac{1}{2}+2(k+\tfrac{1}{2})g_1+(l+\tfrac{1}{2})g_2]\}^2\ , \qquad (1)$$

with $S=1.4915$, $g_1=0.4616$, and $g_2=0.0677$. The integers j are positive, the integers k,l are positive or zero. The zero of energy is taken to be the three-particle breakup threshold throughout the present paper, and atomic units are used. Full quantum-mechanical calculations [2,3] based on the use of Sturmian functions of perimetric coordinates and a complex scaling method have confirmed the very good accuracy of Eq. (1), at least for the case where $k=l=0$.

The states associated with the resonant energy given by Eq. (1) and the condition $k=l=0$ will be described in the present paper as "planetary states" following Ref. [2], for the sake of convenience. These states, within the now usual classification scheme [4] (K,T,N,n), should correspond to K minimum, $K=-N+1$, $T=0$, and $n=N$. The condition $n=N$ does not mean that the degree of excitation of both electrons is similar. The integer number n is only a label that starts from the value N, where N is characterized by the threshold energy $-2/N^2$. Below this, the energy of the states characterized by (K,T,N,n) should converge as n increases to infinity, whereas N remains fixed. When K is maximum $(K=N-1)$ or large, the resonances labeled by $n=N$ are described as intrashell resonances. This term is appropriate because both electrons have the same degree of excitation in that case. In the present case, in which K is minimum, the resonances labeled with $n=N$, i.e., the planetary states, are characterized by quite different degrees of excitation for each electron and should not be called intrashell states.

It is suggested that the energies of the resonances associated with the case $k=l=0$ should converge, as the degree of excitation of both electrons increases, to some of the energies of the resonances associated with the Hamiltonian

$$H=\tfrac{1}{2}p^2+\tfrac{1}{2}p'^2-Z/r-Z/r'+1/||\mathbf{r}|-|\mathbf{r}'|| \qquad (2)$$

in a space where both particles have zero angular momentum ($\ell=\ell'=0$). At present, the Hamiltonian of Eq. (2) is relevant only as far as the resonance energies are concerned. It is clear that the wave functions with $\ell=\ell'=0$ cannot describe electrons localized on the same side of the nucleus.

It is also suggested that each of the terms $(n,k=l=0)$ of the Rydberg series converging to the double-ionization threshold is also the lowest term of another Rydberg series converging to a single ionization threshold of He, and well characterized by a single quantum defect. That means that this series can be described by single-channel quantum-defect theory, and the multichannel quantum-defect theory is not required, at least below the eighteenth threshold. The energies of these Rydberg series of resonances also correspond to the energies of the Rydberg series of resonances associated with the Hamiltonian given by Eq. (2) in a space where both particles have zero angular momentum ($\ell=\ell'=0$).

The analysis of the problem is made within the framework of the method of o(4,2) operator replacements [5]. This method is described very briefly in Sec. II of this work. The basic approximation [Eq. (16)] upon which the present work relies is also given in Sec. II. The implementation of the method of complex scaling for calcu-

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lating resonance energies within the method of o(4,2) operator replacements is first illustrated for the hydrogenic case in Sec. III. The results obtained for the two-electron case are presented and discussed in Sec. IV.

II. BASIC EQUATIONS

The Schrödinger equation for two-electron atoms in the limit of infinite nucleus mass and for nuclear charge Z is

$$(\tfrac{1}{2}p^2 - Z/r + \tfrac{1}{2}p'^2 - Z/r' + 1/|\mathbf{r}-\mathbf{r}'| - E)|\Psi\rangle = 0 \ . \tag{3}$$

The symbols $\mathbf{r}$ and $\mathbf{p}$ denote the position and momentum operators associated with an electron. The superscript prime refers to the other electron. The above equation can be considered within the o(4,2) algebra framework. The method is described in detail in Ref. [5]. The essential points are presented here briefly for the sake of clarity. A realization of the o(4,2) algebra in terms of position and momentum operators has been obtained [6]:

$$\mathbf{a}(\beta) \equiv \exp(-\beta)[\tfrac{1}{2}\mathbf{r}p^2 - \mathbf{p}(\mathbf{r}\cdot\mathbf{p})] - \tfrac{1}{2}\exp(\beta)\mathbf{r} \ ,$$

$$\boldsymbol{\ell} \equiv \mathbf{r}\times\mathbf{p}; \quad \mathbf{g} \equiv r\mathbf{p}; \quad t_2 \equiv r p_r \ ;$$

$$\mathbf{b}(\beta) \equiv \mathbf{a}(\beta) + \exp(\beta)\mathbf{r} \ ,$$

$$t_1(\beta) \equiv \tfrac{1}{2}[\exp(-\beta) r p^2 - \exp(\beta) r] \ ,$$

$$t_3(\beta) \equiv \tfrac{1}{2}[\exp(-\beta) r p^2 + \exp(\beta) r] \ .$$

The o(4,2) operator replacements are the following [5]:

$$r \rightarrow 2\exp(-\beta) t_3(\beta) \ , \tag{4}$$

$$\mathbf{r} \rightarrow -2\exp(-\beta)\mathbf{a}(\beta) \ , \tag{5}$$

$$\mathbf{p} \rightarrow \exp(\beta) t_3^{-1}(\beta)\mathbf{g}/2 \ , \tag{6}$$

$$p^2 \rightarrow \exp(2\beta)[t_3^{-1}(\beta) t_1(\beta) + 1]/2 \ . \tag{7}$$

These replacements are approximations that become exact if the limit β going to $+\infty$ is taken at the end of the calculations or if, for a fixed β value, one considers the limit of zero energy. From now on, for the sake of clarity, we will use the term "replaced problem" for the problem obtained by transforming the original Hamiltonian with the o(4,2) operator replacements [Eqs. (4)–(7)]. The Schrödinger equation, Eq. (1), is transformed[5] into Eq. (8) according to the replacements given by Eqs. (4), (5), and (7):

$$\begin{aligned}[][2T(\beta) + 4(1+\exp(-\beta)\{-[Z/t_3(\beta)] - [Z/t_3'(\beta)] \\ + 1/A(\beta)\}) - 8\exp(-2\beta)E(\beta)] \\ \times [t_3(\beta)t_3'(\beta)]^{1/2}|\Psi(\beta)\rangle = 0 \ ,\end{aligned} \tag{8}$$

$$\begin{aligned}T(\beta) \equiv {} & [t_3(\beta)]^{-1/2} t_1(\beta)[t_3(\beta)]^{-1/2} \\ & + [t_3'(\beta)]^{-1/2} t_1'(\beta)[t_3'(\beta)]^{-1/2} \ ,\end{aligned} \tag{9}$$

$$A(\beta) \equiv |\mathbf{a}(\beta) - \mathbf{a}'(\beta)| \ . \tag{10}$$

$E(\beta)$ and $|\Psi(\beta)\rangle$ denote the eigenvalues and eigenvectors, respectively. The vector

$$[t_3(\beta)t_3'(\beta)]^{1/2}|\Psi(\beta)\rangle$$

is expanded in an orthonormal basis, and one obtains finally an infinite Hermitian matrix for Eq. (8). The basis vectors are labeled by n, n', J_1, and J_2 within a space characterized by the fixed total orbital angular momentum L and its projection M, the total electronic spin S, and the parity π:

$$|(n,n',J_1,J_2,{}^{2S+1}L^{\pi},M)\beta\rangle \ . \tag{11}$$

The basis vectors (11) are defined precisely in terms of scaled hydrogenic vectors, also called Sturmian vectors, in Ref. [5]. The real or complex number β characterizes the scale of length. The wave functions associated with the basis vectors (11) spread over distances of the order of $2n\exp(-\beta)$ for r, and $2n'\exp(-\beta)$ for r'. This clearly indicates that convergence with respect to the size of a truncated basis cannot occur in the limit where the real part of β goes to $+\infty$. The labels n, n', J_1, and J_2 and the good quantum numbers L, S, and π satisfy the conditions [5]

$$\begin{aligned} & n \geq n'; \quad J_1 \geq J_2; \quad J_1 \neq J_2 \ \text{ if } \pi \neq (-1)^L \ ; \\ & n \neq n' \ \text{ if } \pi \neq (-1)^{J_1+J_2+S} \ . \end{aligned} \tag{12}$$

The numbers n and n' are positive integers, and J_1 and J_2 correspond to the coupling of two angular momenta $j=(n-1)/2$, $j'=(n'-1)/2$. Then J_1 and J_2 are coupled and yield L. If the triangular inequalities pertaining to the coupling of angular momenta or the above conditions [Eq. (12)] are not satisfied, the basis vector (11) has to be read as the null vector. Then all the nonzero basis vectors (11) provide a complete orthonormal basis with respect to the $1/(rr')$ scalar product [7]. These basis vectors have eigenvalues $1/n + 1/n'$ with respect to the action of the operator $1/t_3(\beta) + 1/t_3'(\beta)$, and eigenvalues

$$\{2[J_1(J_1+1) + J_2(J_2+1)] - L(L+1)\}^{-1/2}$$

with respect to the action of the operator $1/A(\beta)$ [8,9]. It remains to give the action of the operator $T(\beta)$. The operator $T(\beta)$ satisfies the equation

$$\langle x|T(\beta)|y\rangle = 1/2[\langle x|T_+(\beta)|y\rangle + \langle y|T_+(\beta)|x\rangle^*] \ , \tag{13}$$

and the action of T_+ on the basis vectors is given by Eq. (21) of Ref. [5]. The key point of the present paper is to notice that for $L=0$ and minimum values of J_1 and J_2, i.e., $J_1 = J_2 = (n-n')/2$, Eq. (21) of Ref. [5] is particularly simple.

The following notation is first introduced:

$$|(n,n')\beta\rangle \equiv |[n,n',J_1=\tfrac{1}{2}(n-n') \ , J_2=\tfrac{1}{2}(n-n'), {}^3L^1=0, M=0]\beta\rangle \ . \tag{14}$$

We are considering from now on only triplet S states because the operator $1/A(\beta)$ is not defined for singlet S state [5]. Then Eq. (21) of Ref. [5] gives [10]

$$\begin{aligned}T_+(\beta)|(n,n')\beta\rangle = \alpha(n,n')\{&[(n-n')/(n-n'+1)]^{1/2}[n'/(n'+1)]^{1/2}[1/\alpha(n,n'+1)]|(n,n'+1)\beta\rangle \\ &+[(n-n'+1)/(n-n'+2)]^{1/2}[(n+1)/n]^{1/2}[1/\alpha(n+1,n')]|(n+1,n')\beta\rangle \\ &+(n+1)[(n-n'+2)(n-n'+1)n'(n'+1)]^{-1/2}/\alpha(n,n'+1) \\ &\times|(n,n'+1,J_1+\tfrac{1}{2},J_2+\tfrac{1}{2},{}^{3}0^{1},\beta\rangle\}\ , \end{aligned} \tag{15}$$

where

$$\alpha(a,b)\equiv\begin{cases}\frac{1}{2} & \text{if } a=b \\ (\frac{1}{2})^{1/2} & \text{otherwise}\ .\end{cases}$$

The factors α can be dropped because for the triplet states to be considered, the basis vectors with $n=n'$ have to be read as null vectors [see Eq. (12)]. The minimum value of J_1,J_2 for $L=0$ corresponds to K minimum and $T=0$ in the usual (K,T) classification scheme [4,8,9]. It is stressed, however, that the basis vectors (11) are not hydrogenic ones but are, rather, scaled hydrogenic, with a scaling factor that depends on n,n'.

For $n', n-n'$ sufficiently large, it is seen that the coefficient of the last vector on the right-hand side of Eq. (15) is small with respect to the coefficient of the first two vectors. The basic approximation of this paper is

$$T_+(\beta)\simeq\Theta_+(\beta)\ , \tag{16}$$

with Θ_+ defined by

$$\Theta_+(\beta)|(n,n')\beta\rangle\equiv|(n,n'+1)\beta\rangle+|(n+1,n')\beta\rangle\ . \tag{17}$$

The Hermitic operator $T(\beta)$ is thus approximated by the Hermitic operator $\Theta(\beta)$ defined by

$$\begin{aligned}2\Theta(\beta)|(n,n')\beta\rangle=&|(n,n'-1)\beta\rangle+|(n-1,n')\beta\rangle \\ &+|(n,n'+1)\beta\rangle+|(n+1,n')\beta\rangle\ .\end{aligned} \tag{18}$$

The space spanned by all $|(n,n')\beta\rangle$ vectors remains invariant space for the replaced Schrödinger equation [Eq. (8)] if T is approximated by Θ. The vectors $|(n,n')\beta\rangle$ have the eigenvalues $[(n-n')(n-n'+2)]^{-1/2}$ with respect to the action of $1/A(\beta)$. We also make the approximation

$$1/A(\beta)|(n,n')\beta\rangle\simeq[(n-n')]^{-1}|(n,n')\beta\rangle\ . \tag{19}$$

The conditions of large n' and $n-n'$ for the approximations given by Eqs. (16) and (19) can be justified by physical arguments. First, the decomposition of the resonant state must involve a large value of n' because the spatial extension of the inner electron wave functions, $2n'\exp(-\beta)$, must be large when highly excited resonances are considered. Secondly, $n-n'$ cannot be restricted to small values, because otherwise the terms $1/(n-n')$ would completely dominate the terms $-Z/n-Z/n'$, and the energy would then be above the double ionization threshold. It is then easy to see from Eqs. (18) and (19) and from Eqs. (23) and (24) below that, in the limit where β goes to $+\infty$, the eigenvalue problem becomes equivalent to the eigenvalue problem associated with the Hamiltonian of Eq. (2) in a space where both particles have zero angular momentum ($\ell=\ell'=0$). The approximations discussed above are of the same nature as those that were made in Ref. [11] for the case of maximum J_1,J_2. In that work, a more rigorous mathematical study of this type of approximation was presented. Though we shall not present the details of that work here, we may recall the conclusion: These approximations should improve as the degree of excitation of both electrons increases.

At this point, one could study the Hamiltonian of Eq. (2) by one of the usual methods of quantum mechanics. In Refs. [11,12] the Hamiltonian of Eq. (2) with the term $1/(r+r')$ in place of $1/|r-r'|$ was investigated within the framework of first-order perturbation theory. The present term $1/|r-r'|$ clearly cannot be considered as a perturbation. We choose in the present paper to study the replaced problem with finite β values. The method of o(4,2) operator replacements [5] has been used up to now with real values of the number β, because only bound states were considered. For resonances, it is necessary to use complex β values, as illustrated in the following section.

III. IMPLEMENTATION OF THE METHOD OF COMPLEX SCALING

The numerical diagonalization of a Hermitic Hamiltonian in a truncated basis of order O yields O eigenvalues with possible degeneracy. When the size O of the truncated basis increases without restriction, some of the eigenvalues will converge to the true bound-state energies. However, in an energy range near a resonance, the number of eigenvalues per unit energy increases infinitely with O. The physical reason is that the energy range of a resonance corresponds to the continuum of energies associated with one ionized electron and an ion. In order to locate the resonances energies, specific methods such as the Feshbach projection method or the complex scaling method are then used. Essentially, the complex scaling method amounts to the multiplication of r and p by $\exp(i\theta)$ and $\exp(-i\theta)$ respectively, where θ is a real number. From Eqs. (4)–(7) it is clear that the implementation of the complex scaling method within the method of o(4,2) operator replacement can be made by using complex β values. The method will first be illustrated for the hydrogenic case. For isolated hydrogenic atoms, there are, of course, no resonances. However, it is of interest to consider first this case because it displays conveniently the specific features pertaining to the case of finite complex β values. The Schrödinger equation for a hydrogenic atom is transformed by the o(4,2) operator replacement into the following equation:

$$\{2t(\beta)+2[1-2Z\exp(-\beta)/t_3(\beta)] \\ -8\exp(-2\beta)E(\beta)\}[t_3(\beta)]^{1/2}|\Psi(\beta)\rangle=0\ , \quad (20)$$

$$t(\beta)\equiv[t_3(\beta)]^{-1/2}t_1(\beta)[t_3(\beta)]^{-1/2}\ . \quad (21)$$

$E(\beta)$ and $|\Psi(\beta)\rangle$ denote the eigenvalues and eigenvectors, respectively. The bound-state energies corresponding to Eq. (20) are [5]

$$\varepsilon(\beta,n,Z)=[\exp(2\beta)/4]\{1-[1+(2Z\exp(-\beta)/n)^2]^{1/2}\} \\ =-\tfrac{1}{2}(Z/n)^2\{1-[\exp(-\beta)Z/n]^2 \\ +2[\exp(-\beta)Z/n]^4-\dots\}\ , \quad (22)$$

where n denotes the principal quantum number. It is clear from Eq. (22) that the correct Rydberg hydrogenic value is obtained if the real part of β goes to $+\infty$, or if, for a fixed value of β, one approaches the zero-energy limit ($n\rightarrow\infty$). It is also clear that for finite β values, the bound-state energies become complex if β is complex (with an argument different by $\pm\pi/2$). There is a complete basis of orthonormal vectors that are eigenvectors of t_3 [7]:

$$t_3(\beta)|(n,\ell,m)\beta\rangle=n|(n,\ell,m)\beta\rangle\ . \quad (23)$$

The action of t is given by [7]

$$2t(\beta)|n,\ell,m)\beta\rangle \\ =\{(n+\ell)(n-\ell-1)/[(n-1)n)]\}^{1/2}|(n-1,\ell,m)\beta\rangle \\ +\{(n+\ell+1)(n-\ell)/[(n+1)n]\}^{1/2} \\ \times|(n+1,\ell,m)\beta\rangle\ . \quad (24)$$

In the above equation, the vector $|(n=0,\ell=0,m=0)\beta\rangle$ has to be read as the null vector. If the vector

$$t_3(\beta)^{1/2}|\Psi(\beta)\rangle$$

is expanded in this orthonormal basis, one obtains a tridiagonal infinite matrix eigenvalue problem which has Eq. (22) as solutions. Figure 1 reports the numerical results obtained for the case of $\ell=0$ with the truncated basis involving one hundred vectors ($n=1-100$), $\beta=0-0.1i$, $Z=1$. The abscissa corresponds to the real part of the energy, the ordinate to the imaginary part. The relative accuracy with respect to the exact results given by Eq. (22) is better than or of the order of 10^{-11} for the first six eigenvalues, and then decreases rapidly. Thus, it is only of the order of 10^{-5} for the eighth eigenvalue. It is seen in this figure that, as usual, the continuum spectrum is rotated by an angle corresponding to the argument of 2β. It can be shown [13] that the operator $\exp(2\beta)[1+t(\beta)]/4$, which is associated with the kinetic energy, is bounded by $\frac{1}{2}\exp(2\beta)$. This continuum appears in Fig. 1 as a discrete set of points due to the finite size of the matrix. These points are not exactly located on a straight line due to the finite size of the matrix. The finite size of the matrix is also apparent in Fig. 1 because the Rydberg series is represented only by a finite number of terms. The negative-energy terms close to zero energy, corresponding to the top of the vertical line of Fig. 1, have not converged, or are missing. It is of interest to note that if the same numerical calculation is repeated but for a different value of β, $\beta=-1\ -0.1i$, then the agreement with respect to Eq. (22) is better than or of the order of 10^{-11} for the first 11 eigenvalues. This illustrates the fact that for a fixed size of the truncated basis ($n\leq O$), the agreement with the exact results given by Eq. (22) improves as the real part of β decreases. In the limit where the real part of β goes to $-\infty$, it can be seen from Eq. (20) that the basis vectors $|(n,l,m)\beta\rangle$ become exact eigenvectors with eigenvalues

$$\varepsilon(\beta,n)\simeq\exp(\beta)Z/(2n)\ . \quad (25)$$

Before turning to the two-electron atomic problem in Sec. IV, the different kind of convergences to be considered will be described. The first kind is the convergence of the solutions of the replaced problem with respect to the solutions of the original problem. This case has to be divided into two subcases. First, the convergence of a given eigenvalue when the real part of β goes to $+\infty$; secondly, for a fixed β value, the convergence of the replaced eigenvalues towards the original eigenvalues when one moves towards the zero-energy limit. It is essentially this latter convergence that will be of interest in Sec. IV. The second kind of convergence to be considered is the convergence of the replaced problem with respect to the size of a truncated basis including all basis vectors with n smaller than a given integer O. This convergence improves as the real part of β decreases, as illustrated previously.

IV. NUMERICAL RESULTS

We now turn to the study of the eigenvalues $E(\beta)$ of Eq. (8) within the approximations given by Eqs. (16)–(19). In the limit where the real part of β goes to $+\infty$, or, for a fixed β value, in the limit of zero energy, this problem should correspond to the study of the Hamiltonian given by Eq. (2) in the space where both particles have zero angular momentum ($\ell=\ell'=0$). We consider a truncated basis involving all basis vectors with n,n' ($n>n'$) smaller or equal to a given value O. The size of this basis is thus equal to $O(O-1)/2$. The matrix eigenvalue problem then is of band type, since the only nonzero diagonal elements originate from the operator Θ, whose action on the basis vectors is given by Eq. (18). Thus the nonzero nondiagonal elements are all equal to unity. The algorithm used for computing eigenvalues is the Lanczos algorithm without reorthogonalization procedures, as described in Refs. [14,15]. Numerical calculations were performed for five different β values: $0-0.1i$, $-0.25-0.1i$, $-0.5-0.1i$, $-0.75-0.1i$, and $-1-0.1i$. The value for O is 100. The results for the value β $0-0.1i$ are displayed in Fig. 2. It is seen in this figure that a series of resonances approach from the left each single ionization threshold [Eq. (22), with $Z=2$].

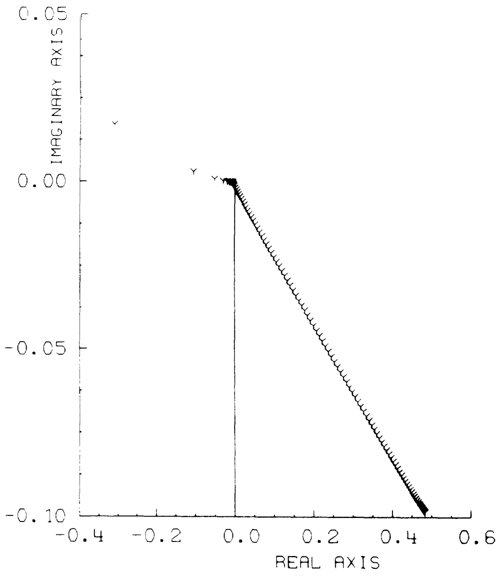

FIG. 1. Energies from numerical diagonalization of the tridiagonal matrix of order 100 ($1 \leq n \leq 100$) associated with the replaced hydrogenic problem [see Eqs. (20)–(24)]. $Z=1$, $l=0$, $\beta = 0-0.1i$.

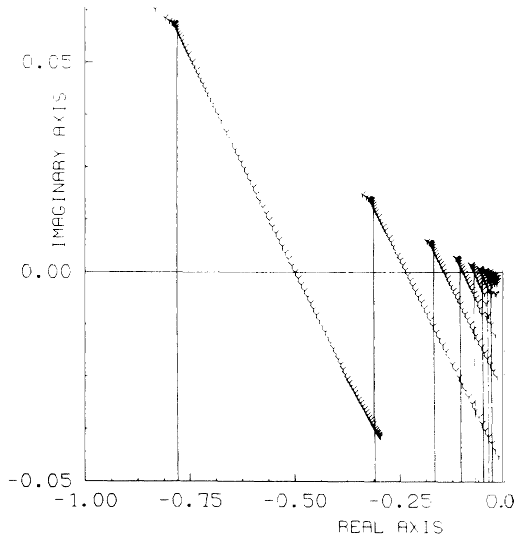

FIG. 2. Energies from numerical diagonalization of the band matrix of order 4950 ($1 \leq n' < n \leq 100$) associated with the replaced approximated two-electron problem [see Eqs. (8) and (16)–(19)]. $Z=2$, $\beta = 0.-0.1i$. The first eight thresholds $\varepsilon(\beta, N=1-8, Z=2)$ [see Eq. (22)] are reported as the top of the first eight vertical lines. The last vertical line corresponds to the double ionization threshold (zero of energy).

We now consider the first (i.e., the one with the smallest real part of the energy) resonance of each series converging to the different thresholds. The real part of the ratio of the first resonance energy below each threshold to the energy of the same threshold is reported on Table I. The imaginary part of this ratio is of the order of 10^{-4}. These ratios are also reported on Fig. 3 as a function of the real part of the threshold energies $\varepsilon(\beta, N, Z=2)$ given by Eq. (22). Within the errors intrinsic to any extrapolation process, it can be seen that these ratios converge to about 1.11 in the limit of zero energy, i.e., in the limit of high excitation of both electrons, where the present model should be relevant for the resonance energies of the real helium atom. The ratios $E/[-4/(2N^2)]$ for the helium atom, calculated with the values reported in Ref. [2] for E, are, for N increasing between 3 and 11, 1.1248, 1.1207, 1.1183, 1.1167, 1.1157, 1.1150, 1.1145, 1.1142, and 1.1139. [It should be noted that the j of Eq. (1) of the present paper corresponds to $N-1$, where N labels the single ionization threshold.] The ratio derived from the semiclassical equation (1) [2] is $(1.4915)^2/2 = 1.112$ in the limit of infinite quantum numbers. Thus, the value 1.11 obtained from the present paper reproduces within about one percent the quantum results obtained in Ref. [2].

The accuracy of the present results is far from the extraordinary accuracy obtained in Ref. [2]. In particular, the accuracy is not sufficient enough to give information on the width of the resonances. Nevertheless, the present approach brings two important qualitative results to light. First, this approach shows how the energies of the so-called planetary states can be described by a quantum

TABLE I. The first line gives the real part of β. The imaginary part of β is always equal to -0.1. The first column labels the single ionization thresholds $\varepsilon(\beta, N, Z=2)$ given by Eq. (22). The other columns report, for a given β value, the real part of the ratio of the lowest resonance energy of the Rydberg series converging to a threshold by the energy of this threshold.

$N \backslash \beta$	0.00	-0.25	-0.50	-0.75	-1.00
1	1.0686	1.0698	1.0708	1.0718	1.0728
2	1.0853	1.0851	1.0846	1.0840	1.0834
3	1.0937	1.0937	1.0931	1.0920	1.0907
4	1.0982	1.0986	1.0984	1.0975	1.0960
5	1.1008	1.1014	1.1016	1.1012	1.0999
6		1.1032	1.1037	1.1036	1.1028
7			1.1050	1.1053	1.1048
8				1.1064	1.1063

TABLE II. Real part of the effective quantum number ν as defined by Eq. (26), where E results from numerical diagonalization for the case $\beta=0-0.1i$.

Threshold	Real part of ν for $\beta=0-0.1i$						
1	2.90	3.92	4.94	5.94	6.95	7.95	8.95
2	4.24	5.26	6.27	7.27	8.28	9.28	
3	5.57	6.58	7.58	8.59			
4	6.94	7.94	8.95				
5	8.34	9.35					

problem with only two degrees of freedom in the limit of high excitation. Second, the energy of each planetary state appears as the lowest member of a well-defined Rydberg series of resonances converging to single ionization thresholds. In order to see how these series are indeed characterized by a single quantum effect, Table II details, for $\beta=0-0.1i$, the effective quantum number of the series calculated from the equation

$$E=\varepsilon(\beta,N,2)+\varepsilon(\beta,\nu,1)\ , \qquad (26)$$

where E are the numerical results reported in Fig. 1. As E is complex, ν is also complex, but the imaginary part of ν is small (less than 0.1) and approximately constant within a given Rydberg series. It is clear from Table II that the real part of ν increases by nearly one unit at each new resonance of the series. The numerical values of these effective quantum numbers are of no physical meaning, since the limit of the infinite real part of β should be taken. The fact that these effective quantum numbers increase by a step of almost one unit, however, clearly characterizes an unperturbed Rydberg series. An approximate value for the effective quantum number of the lowest terms of the Rydberg series in the helium case can be obtained by comparing the semiclassical equation (1) with Eq. (26), $j=N-1$. One obtains approximately $\nu=1.49N$. The fractional part of this effective quantum number should vary slowly when one goes to higher Rydberg states of a given series, and then stabilize. Multichannel quantum-defect theory, however, could become necessary above the energy range where different Rydberg series being to overlap. From Eq. (1), this situation begins when $-[1.4915/(N+1)]^2<-2/(N^2)$, i.e., above the 18th threshold.

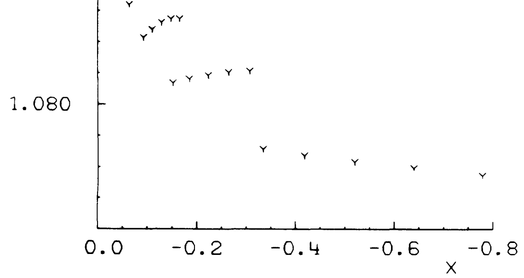

FIG. 3. The real parts of the ratios reported in Table I are displayed (y axis) as a function of the real part of the thresholds energies $\varepsilon(\beta,N,Z=2)$ given by Eq. (22) (x axis).

V. CONCLUDING REMARKS

The classical problem of two electrons moving on the same rectilinear trajectory, on the same side of the nucleus, is basically a problem with two degrees of freedom. A remarkable result of Ref. [1] is the existence of stable motions. Here, we start from a purely quantum approach and use the method of o(4,2) operator replacements. We found that, within some approximations, some solutions of the replaced problem can be described in subspaces of the whole Hilbert space. These subspaces are spanned by the vectors of Eq. (14) involving only two independent integer labels (n,n'). These vectors involve many different values of angular momentum quantum numbers ℓ,ℓ' of each electron. The concrete form of the replaced Hamiltonian matrix in the sub-bases spanned by the vectors of Eq. (14) is, however, the same as for the replaced problem corresponding to the Hamiltonian of Eq. (2), in the space where $\ell=\ell'=0$.

The present estimations for the energy resonances of the planetary states agree with the very accurate full quantum results of Refs. [2,3]. This supports the approximations upon which the present work relies, and, in our opinion, also supports the existence of nearly unperturbed Rydberg series above each of the planetary states that appear in the present calculations.

This paper presents an illustration of the method of o(4,2) operator replacement for the study of resonances. Clearly, the method is not competitive with the method of Ref. [2] as long as precise energy values are required. It has, however, the advantage of producing without optimization procedure and within a single numerical diagonalization (one for each distinct β value) a global picture of the resonance spectrum.

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