

Doubly excited P^e and D^o Feshbach resonances in the lithium isoelectronic sequence

Mirosław Bylicki

*Instytut Fizyki, Uniwersytet Mikołaja Kopernika, ul. Grudziądzka 5, 87-100 Toruń, Poland**
and Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation,
48 Vassileos Constantinou Avenue, 11635 Athens, Greece[†]

(Received 2 July 1992)

The Feshbach projection method and the generalized saddle-point technique have been used to obtain energies of $4,2P^e$ and $4,2D^o$ Feshbach resonances in He^- , Li , and Be^+ . The results from both methods confirm each other. Positions and Auger energies of 31 resonances (3 in He^- , 14 in Li , and 14 in Be^+) lying between the 2^1P^o and 3^3P^o thresholds are given. These data can serve as a basis for identification of those resonances in future experiments. Some suggestions for such experiments are made.

PACS number(s): 31.50.+w, 32.80.Dz

I. INTRODUCTION

Continua of the P^e , D^o , F^e , etc. symmetries of three-electron atomic systems start at the 2^3P^o two-electron threshold. Therefore all the states of these symmetries having energies below that threshold are metastable against Coulomb autoionization. They have been investigated theoretically [1,2] and experimentally [3,4]. On the other hand, resonances of those symmetries, lying above the 2^3P^o threshold, have not yet been investigated, except for the $1s2p2p^4P^e$ shape resonance in He^- and the $1s3p3p^4P^e$ Feshbach resonance in the lithium isoelectronic sequence. The former has been treated experimentally by Peterson, Coggiola, and Bae [5] and theoretically by Nicolaides and Komninos [6]. The existence of the latter has been predicted by calculations of Davis and Chung [7]. It seems that resonances of the above-mentioned symmetries have been of minor interest because they are more difficult to observe than the ones most investigated $2S^e, 2P^o, 2D^e$, etc. They cannot be seen in electron scattering on the two-electron target in the ground or metastable 2^3S^e state, nor can they be excited from the ground three-electron state by electric dipole absorption. They are also experimentally more difficult than their bound counterparts because, being autoionizing resonances, they are hard or even impossible to observe in emission. In principle, nevertheless, experiments in which these resonances could be observed are possible. For instance, they could be identified by means of the spectroscopy of the Auger electrons emitted by species excited in collisions with heavy ions or in beam-foil collisions [8]. Optical absorption experiments involving doubly excited bound states as the initial ones are also possible. Therefore in this work we pay attention to those states, aiming at predicting positions (energies) of $4,2P^e$ and $4,2D^o$ Feshbach resonances lying between the 2^1P^o and 3^3P^o thresholds, in the lithium isoelectronic sequence for $Z=2-4$.

To obtain the resonant energies we have used the QHQ approximation of the Feshbach-projection operator method [9] in the formulation given by Bylicki [10]. The QHQ method is known as providing good approxima-

tions to the energies of closed-channel (Feshbach) resonances. However, because of the lack of experimental data for comparison, we have used additionally the generalized saddle-point (GSP) method [11], in order to check whether variation of open-channel description can change the results significantly, i.e., in order to test the reliability of our results. Both methods are briefly presented in Sec. II. The results are given in Sec. III.

II. METHODS OF CALCULATION

A. QHQ method

Resonant-state energies are obtained from the QHQ method as eigenvalues of the QHQ operator. H is the N -electron nonrelativistic Hamiltonian. The projection operator Q corresponds to a closed-channel space and is the complement of the projector P ($P+Q=1$) projecting onto the open-channel space according to

$$P\Psi = \sum_{\nu} \mathcal{A}\psi_{\nu}(r^{(N)})u_{\nu}(r_N), \quad (1)$$

where $\psi_{\nu}(r^{(N)})$ is a channel wave function in which the $(N-1)$ -electron target-state wave function ϕ_i is coupled to the angular momentum l and spin of the incoming (or outgoing) electron, as defined by Temkin and Bhatia [12] and applied in Ref. [10]. The summation in Eq. (1) is taken over $\nu=(i,l)$ corresponding to the open channels only, i.e., $i \leq M$ (M is the number of open channels). We do not use the explicit form of P . Instead, we notice that if a configuration-interaction-type wave function Ψ is to be projected and if the target-state wave functions ϕ_i , $i \leq M$, are also of configuration-interaction type, then the u_{ν} functions are strictly expressible as linear combinations of orbitals φ_k occurring in Ψ and ϕ_i , $i \leq M$. Coefficients $U_{\nu j}$ of these expansions are found as a solution of the system of linear algebraic equations:

$$\begin{aligned} & \langle \psi_{\mu}(r^{(N)})\varphi_k(r_N) | \Psi \rangle \\ &= \sum_{\nu, j} \langle \psi_{\mu}(r^{(N)})\varphi_k(r_N) | \mathcal{A}\psi_{\nu}(r^{(N)})\varphi_j(r_N) \rangle U_{\nu j} \end{aligned} \quad (2)$$

for all μ and k for which $\mathcal{A}\psi_{\mu}\varphi_k \neq 0$. Equation (2) is equivalent to the requirement of idempotency of P and Q .

If the QHQ method is to be practically applied, two elements have to be defined in detail: the target-state wave functions ϕ_i and the trial function Ψ . They are described below as they have been used in this work.

1. Target-state wave functions

There are two open channels which should be taken into account when considering the Feshbach ${}^2P^e$ and ${}^2D^o$ resonances of a three-electron atom, lying between the $2\,{}^1P^o$ and $3\,{}^3P^o$ target thresholds. They are associated with the $2\,{}^3P^o$ and $2\,{}^1P^o$ two-electron states. In the case of ${}^4P^e$ and ${}^4D^o$ resonances the $2\,{}^3P^o$ target state constitutes the only open channel. The one-configuration $(1s2p)^3P^o$ and $(1s2p)^1P^o$ functions have been used as approximations to the wave functions of these target states. They have been constructed in terms of Slater-type orbitals (STO's) with the exponents optimized so as to minimize the energies of $2\,{}^3P^o$ and $2\,{}^1P^o$ states of the isolated target. Their optimal values together with the corresponding energies are given in Table I.

2. Trial function

The trial function Ψ has been taken in a configuration-expansion form using Slater-type orbitals. Several angular terms of the $[(l_1, l_2)l_{12}, l_3]$ type have been used for each symmetry under consideration. These were $[(s, p)P, p]$, $[(s, d)D, d]$, $[(s, f)F, f]$, $[(p, p)P, d]$, $[(p, p)D, d]$, and $[(p, d)D, f]$ for the P^e total symmetry, and $[(s, p)P, d]$, $[(s, d)D, f]$, $[(p, p)P, p]$, and $[(p, d)P, d]$ for the D^o total symmetry. In the case of doublets both triplet and singlet intermediate couplings have been used. For the quartets the singlet intermediate coupling has been obviously excluded. The nonlinear parameters (exponents of STO's) have been associated with the angular terms. Thus, in principle, all the radial terms belonging to a given angular term have been used with the same parameters, in particular the singlet and the triplet intermediate-coupling terms have had the same nonlinear parameters. However, some angular terms have appeared in the trial expansion twice or even three times with various sets of nonlinear parameters.

In order to minimize the computational effort a common basis set has been used for all the resonances of a

given spin-angular symmetry, of a given Z . Accordingly, the nonlinear parameters have been optimized so as to minimize the sum of the energies of all the resonances under consideration and not to minimize each of them individually.

B. Generalized saddle-point method

The GSP method has been proposed [11] as a generalization of the saddle-point technique [13] and a link connecting the latter one with the Feshbach projection-operator method [9]. Commentaries on saddle-point methods have recently been given in the literature [14]. The GSP method is based on the minimax principle [15]. The latter holds strictly only for the discrete spectrum of a Hermitian operator. A justification of its application to resonant state energies has been given in Ref. [11]. In this work we are studying several lowest-lying resonances of a given symmetry at once. The mini-max principle adapted for such a case reads

$$\sum_{i=1}^m E_{\text{GSP}_i} = \sup_{\mathcal{P} \subset \mathcal{D}_m} \inf_{\mathcal{D}_m \subset \mathcal{P}^\perp} \text{Tr}_{\mathcal{D}_m} H, \quad (3)$$

i.e., in order to gain the sum of energies $E_{\text{GSP}_1}, \dots, E_{\text{GSP}_m}$ corresponding to m lowest-lying Feshbach resonances, one should minimize the trace of H in an m -dimensional subspace \mathcal{D}_m orthogonal to a space \mathcal{P} , corresponding to open channels, varying the subspace \mathcal{P} so as to maximize the trace of H in \mathcal{D}_m .

In order to see clearly the relation between the QHQ and GSP methods, it is convenient to write the essential idea of the QHQ method (as described above) in a form similar to Eq. (3):

$$\sum_{i=1}^m E_{\text{QHQ}_i} = \inf_{\mathcal{D}_m \subset \mathcal{P}^\perp} \text{Tr}_{\mathcal{D}_m} H, \quad (4)$$

where \mathcal{P} is not to be varied; it is determined by ϕ_i optimal for the isolated target [as defined in Eq. (1); the approximate ϕ_i used in this work are given in Table I]. Thus the GSP technique differs from the QHQ method only by the maximization of the resonance energies with respect to the target-state description used within the open-channel space representation. In this work the GSP calculation has been realized using the same trial function and the same open-channel-space form as those used within the QHQ computations. The GSP-method maximization has been performed with respect to the exponents of STO's used within the $(1s2p)^3P^o$ and $(1s2p)^1P^o$ target-state approximations. The optimal values of the STO exponents shall be given in Sec. III together with the corresponding resonance energies.

III. RESULTS AND DISCUSSION

Both the QHQ and GSP calculations have been performed for He^- , Li , and Be^+ . Quartets as well as doublets of the P^e and D^o symmetries have been considered. Three Feshbach resonances have been found in He^- : one of each ${}^4P^e$, ${}^2D^o$, and ${}^2P^e$ symmetry. For Li and Be^+ our calculations have been confined to four lowest doublets

TABLE I. Target-state approximations.

Z	State	Nonlinear parameters		Energy (a.u.)
		1s	2p	
2	$(1s2p)^3P^o$	1.991	0.544	-2.1307
	$(1s2p)^1P^o$	2.000	0.482	-2.1224
3	$(1s2p)^3P^o$	2.98	1.082	-5.0232
	$(1s2p)^1P^o$	3.007	0.97	-4.9900
4	$(1s2p)^3P^o$	3.97	1.60	-9.1696
	$(1s2p)^1P^o$	4.008	1.465	-9.1061

TABLE II. The energies (in a.u.) of ${}^4P^e$ resonances.

Z	State	$-E_{QHQ}$	$-E_{GSP}$	q_{1s}	q_{2p}	M	N	R
2	$1s3p3p$	2.065 013	2.064 360	1.364	0.484	6(8)	18	53
3	$1s3p3p$	4.848 352	4.846 044	2.21 ^a	1.015 ^a	5(9)	18	89
	(2)	4.792 586	4.792 427	2.314 ^b	1.135 ^b			
	(3)	4.779 723	4.778 797					
4	$1s3p3p$	8.855 215	8.852 557	4.0 ^a	1.525 ^a	5(9)	18	88
	(2)	8.758 243	8.757 930	3.995 ^b	1.705 ^b			
	(3)	8.677 194	8.676 192					

^aThe values of q parameters for the first and the third ${}^4P^e$ states.

^bThe values of parameters for the second ${}^4P^e$ resonance.

and three lowest quartets of P^e and D^o symmetries. The obtained energies of these states are given in Tables II–V. Information concerning basis sets used is also given. M is the number of different angular terms; in parenthesis the number of groups of configurational functions differing by nonlinear parameters is given. N is the number of nonlinear parameters which have been optimized, and R is the total number of radial terms, i.e., the number of linear coefficients. The information concerning basis sets is common for all the resonant levels of a given symmetry for a given Z . In addition, the exponents (q parameters) of the target open-state orbitals, for which the GSP energies have been obtained, are given. As one can see, the D^o energies are not very sensitive to the changes of target-state parameters: the QHQ and GSP energies do not differ very much. This is not the case for the P^e states. The lowest P^e resonance energies depend strongly on q parameters. Moreover, they reach the maximum at different values of q than the higher ones do. Therefore, the maximization of the sum of all energies caused a slight lowering of higher roots. Though this is allowed by the mini-max principle, the computations have been completed by additional maximization: the second ${}^4P^e$

root has been maximized individually and the sum of the second and third ${}^2P^o$ roots (for $Z=3$ and 4). This additional optimization has shown that these roots are not very sensitive to the variation of q 's.

It is useful to characterize atomic states by the leading electronic configurations. Unfortunately, this cannot be determined definitely in this work because of the use of nonorthogonal basis sets. However, since the Feshbach projection removes from the trial function the $1s2p$ core, the resonances under consideration are of $1s3pnl$ ($n \geq 3$, $l=p,d$) type. One can guess that the lowest quartet and doublet P^e resonances should be assigned to the $1s3p3p$ configuration and the lowest quartet and doublet D^o resonances to the $1s3p3d$ configuration. Three lowest ${}^4D^o$ resonances can be presumably assigned to the $1s3p3d$, $1s2p4d$, and $1s2p5d$ configurations. It is rather difficult to guess the configurational designation of the remaining resonances because of two possible intermediate couplings in case of doublets, and possible perturbation of the P^e states by the $1s3d^2$ configuration. Therefore in the tables only the ${}^4D^o$ resonances and the lowest ones in each symmetry are configurationally characterized. The remaining ones are only numbered.

TABLE III. The energies (in a.u.) of ${}^2P^e$ resonances.

Z	State	$-E_{QHQ}$	$-E_{GSP}$	q_{1s} ^a	q_{2p} ^a	M	N	R
2	$1s3p3p$	2.059 635	2.058 766	2.204	0.500	6(8)	17	104
				2.202	0.416			
3	$1s3p3p$	4.811 340	4.805 283	3.028 ^b	0.995 ^b	5(9)	17	133
	(2)	4.789 710	4.788 683	3.026	0.865			
	(3)	4.782 635	4.782 343	3.028 ^c	1.029 ^c			
	(4)	4.763 584	4.763 018	3.028	0.926			
4	$1s3p3p$	8.778 446	8.771 334	4.007 ^b	1.45 ^b	5(9)	17	140
	(2)	8.732 508	8.712 553	4.005	1.31			
	(3)	8.684 712	8.684 237	4.004 ^c	1.563 ^c			
	(4)	8.643 177	8.643 146	4.005	1.453			

^aThe upper values correspond to the $(1s2p)^3P^o$ target state and the lower ones to the $(1s2p)^1P^o$ state.

^bThe values of q parameters for the first two ${}^4P^e$ resonances.

^cThe values of q parameters for the third and the fourth ${}^4P^e$ resonances.

TABLE IV. The energies of ${}^4D^o$ resonances.

Z	State	$-E_{QHQ}$	$-E_{GSP}$	q_{1s}	q_{2p}	M	N	R
3	$1s3p3d$	4.820 356	4.820 051	2.38	1.040	4(7)	16	86
	$1s3p4d$	4.780 723	4.780 553					
	$1s3p5d$	4.765 653	4.765 553					
4	$1s3p3d$	8.807 819	8.807 337	4.023	1.549	4(7)	16	89
	$1s3p4d$	8.679 289	8.679 007					
	$1s3p5d$	8.650 437	8.650 267					

To our knowledge the resonances presented here have not been observed. They cannot be seen in an electron scattering on a target in the ground 1^1S or in the metastable 2^3S state, or in the synchrotron-radiation absorption from the ground state of three-electron system. All of them, however, could be populated by collisions with heavy ions or in beam-foil experiments [8]. The other possibility is an optical-absorption experiment in which the resonant states could be obtained by electric dipole transition from doubly excited states metastable against autoionization. In He^- , $1s2s2p^4P^o$ is the only such state, and only a ${}^4P^e$ resonance can be excited from it. The $1s2p2p'^4P^e$ shape resonance has been measured in such a way by Peterson, Coggiola, and Bae [5]. Very recently Träbert *et al.* [16] have observed this resonance in emission from the $2p^3^4S^o$ metastable state. The latter work was preceded by theoretical prediction of Nicolaides and Komninos [6] and Nicolaides [17], and is the first experimental confirmation of the $2p^3^4S^o$ state as first predicted by Beck and Nicolaides [18]. One may hope that the Feshbach ${}^4P^e$ resonance presented here can also be observed in a similar way.

In Li and Be^+ the variety of doubly excited metastable states from which our resonance could be optically excited is greater. Moreover, since our resonances should be considered as being of the $1s3pnl$ ($n \geq 3$) type, then the $E1$ transition probabilities for the absorption from the $1s2p3p^2P^e$ and ${}^4P^e$ or $1s2s3p^4P^o$ states should be large enough to make the measurements possible. The only

problem one can expect to appear is for the ${}^2P^e$ states which need excitation of two electrons to be obtained from the doubly excited $1s2pnd^2D^o$ states. Fortunately, combination of lasers with synchrotron radiation opens another possibility for those states. Li or Be^+ can be excited to the $1s3pnp^2P^e$ resonances by absorption of synchrotron radiation from singly excited $1s^2np^2P^o$ states obtained earlier by pumping the $1s^22s^2S^e \rightarrow 1s^2np^2P^o$ transitions using a laser. For ${}^2D^o$ resonances such an experiment is also thinkable, but more complicated. Two lasers would be needed to prepare the $1s^2nd^2D^e$ state from which the $1s3pnd^2D^o$ resonances could be reached by synchrotron-radiation absorption. The above speculations constitute some suggestions for the future experiments, although they should be confirmed by computation of the transition probabilities and the lifetimes of the initial states, to be more definite.

Regardless of the way in which the resonances under consideration are populated they will decay mainly by Coulomb autoionization. For the doublets two channels associated with the 2^3P^o and 2^1P^o target states are open. For the quartets there is only one: 2^3P^o . Corresponding Auger energies $\Delta E(2^3P^o)$ and $\Delta E(2^1P^o)$ are displayed in Tables VI–VIII. As many decimal figures are given as is necessary to see the difference between the QHQ and the GSP results. We do not claim, however, our results to be of 1-meV accuracy. Neither the energy shift caused by interaction with the continua nor the relativistic effects have been taken into account in the present computa-

TABLE V. The energies (in a.u.) of ${}^2D^o$ resonances.

Z	State	$-E_{QHQ}$	$-E_{GSP}$	q_{1s}^a	q_{2p}^a	M	N	R	
2	$1s3p3d$	2.060 908	2.060 582	1.804	0.490	5(6)	16	80	
				1.205	0.428				
3	$1s3p3d$	4.834 364	4.833 486	3.14	1.025	3(6)	13	153	
				3.36	0.947				
				(2)	4.815 254				4.815 154
				(3)	4.777 597				4.777 533
(4)	4.772 243	4.772 154							
4	$1s3p3d$	8.830 405	8.829 081	4.025	1.533	3(6)	13	142	
				4.01	1.439				
				(2)	8.796 304				8.796 179
				(3)	8.673 610				8.673 483
				(4)	8.663 469				8.663 340

^aThe upper values correspond to the $(1s2p)^3P^o$ target state and the lower ones to the $(1s2p)^1P^o$ state.

TABLE VI. The lowest ${}^4P^e$ ${}^2D^o$, and ${}^2P^e$ resonances in He^- . Positions ΔE and Auger energies $\Delta E(2^3P^o)$ and $\Delta E(2^1P^o)$ are calculated in eV (1 a.u.=27.2079 eV), with respect to the non-relativistic He ground-state level and the 2^3P^o and 2^1P^o levels taken from Refs. [19] and [20], respectively.

Resonance	ΔE	$\Delta E(2^3P^o)$	$\Delta E(2^1P^o)$
$1s3p3p\ {}^4P^e$	22.82	1.85	
	22.84	1.87	
$1s3p3d\ {}^2D^o$	22.93	1.966	1.71
	22.94	1.975	1.72
$1s3p3p\ {}^2P^e$	22.97	2.00	1.75
	22.99	2.02	1.77

TABLE VII. P^e and D^o resonances in Li. Positions ΔE (in eV) are given with respect to the nonrelativistic Li ground state taken from Ref. [21], and the Auger energies $\Delta E(2^3P^o)$ and $\Delta E(2^1P^o)$ are calculated using the nonrelativistic Li^+ 2^3P^o and 2^1P^o levels taken from Ref. [20] (1 a.u.=27.2095 eV).

Resonance	ΔE	$\Delta E(2^3P^o)$	$\Delta E(2^1P^o)$
$1s3p3p\ {}^4P^e$	71.55	4.88	
	71.62	4.94	
$1s3p3d\ {}^2D^o$	71.93	5.26	4.33
	71.96	5.28	4.35
$1s3p3d\ {}^4D^o$	72.315	5.64	
	72.323	5.65	
${}^2D^o(2)$	72.454	5.781	4.846
	72.456	5.784	4.849
$1s3p3p\ {}^2P^e$	72.6	5.9	5.0
	72.7	6.0	5.1
${}^4P^e(2)$	73.071	6.398	
	73.075	6.402	
${}^2P^e(2)$	73.15	6.48	5.54
	73.18	6.50	5.57
${}^2P^e(3)$	73.34	6.67	5.73
	73.35	6.68	5.74
$1s3p4d\ {}^4D^o$	73.393	6.721	
	73.398	6.725	
${}^4P^e(3)$	73.42	6.75	
	73.45	6.77	
${}^2D^o(3)$	73.478	6.806	5.871
	73.480	6.807	5.872
${}^2D^o(4)$	73.624	6.951	6.016
	73.626	6.954	6.019
$1s3p5d\ {}^4D^o$	73.803	7.131	
	73.806	7.133	
${}^2P^e(4)$	73.86	7.19	6.25
	73.88	7.20	6.27

tions. The calculation of Davis and Chung [7] for the $1s3p3p\ {}^4P^e$ resonances has shown that those effects are less than the differences between the *QHQ* and GSP results. Thus we can suppose that the accuracy of the present results is about few tens of meV, in general, and about several tenths of eV for the lowest two ${}^2P^e$ states in Be^+ . We do not consider the *QHQ* results or the GSP ones to be better than the others. The GSP calculations have been performed not in order to obtain better results, but rather to see how the results change with respect to the variation of the target description. It has been found that this dependence is not very strong; the sequence of

TABLE VIII. P^e and D^o resonances in Be^+ . ΔE , $\Delta E(2^3P^o)$, and $\Delta E(2^1P^o)$ are, respectively, the position calculated with respect to the nonrelativistic Be^+ ground level [2] and the Auger energies calculated using the nonrelativistic energies of the Be^{2+} 2^3P^o and 2^1P^o states as given in Ref. [20] (1 a.u.=27.2100 eV).

Resonance	ΔE	$\Delta E(2^3P^o)$	$\Delta E(2^1P^o)$
$1s3p3p\ {}^4P^e$	148.83	8.70	
	148.90	8.77	
$1s3p3d\ {}^2D^o$	149.50	9.38	7.63
	149.54	9.41	7.66
$1s3p3d\ {}^4D^o$	150.12	9.99	
	150.13	10.00	
${}^2D^o(2)$	150.431	10.304	8.557
	150.434	10.307	8.560
$1s3p3p\ {}^2P^e$	150.9	10.8	9.0
	151.1	11.0	9.2
${}^4P^e(2)$	151.47	11.34	
	151.48	11.35	
${}^2P^e(2)$	152.2	12.0	10.3
	152.7	12.6	10.8
${}^2P^e(3)$	153.47	13.34	11.59
	153.48	13.35	11.61
$1s3p4d\ {}^4D^o$	153.615	13.488	
	153.622	13.495	
${}^4P^e(3)$	153.67	13.54	
	153.70	13.57	
${}^2D^o(3)$	153.769	13.642	11.895
	153.773	13.646	11.899
${}^2D^o(4)$	154.045	13.918	12.171
	154.049	13.922	12.175
$1s3p5d\ {}^4D^o$	154.400	14.273	
	154.404	14.277	
${}^2P^e(4)$	154.597	14.470	12.723
	154.598	14.471	12.724

TABLE IX. The Auger energies $\Delta E(2^3P^o)$ (in eV) for the $1s3p3p^4P^e$ resonances in the lithium isoelectronic sequence. Comparison with the Davis-Chung [7] results.

Z	Davis and Chung	This work	
		QHQ	GSP
2	1.854	1.85	1.87
3	4.925 36	4.88	4.94
4	8.777 70	8.70	8.77

the resonances has been not influenced by the maximization of the GSP method. The resonances are well separated and the positions of them are determined unambiguously.

The only data in the literature we can compare our results with are the Auger energies calculated by Davis and Chung [7] for the lowest $^4P^e$ resonances. The comparison is given in Table IX. Keeping in mind that in their com-

putations Davis and Chung [7] have taken into account the relativistic corrections and the continuum shift, one can state that the agreement is very good.

In conclusion, we state that using the QHQ approximation of the Feshbach-projection method and the generalized saddle-point method we have obtained positions of 31 P^e and D^o Feshbach resonances lying between the 2^1P^o and 3^3P^o thresholds, in He^- , Li, and Be^+ . Only three of those states have been considered previously by Davis and Chung [7]. The results obtained in this work, although they do not contain relativistic or continuum-interaction contributions, are in satisfactory agreement with the Davis and Chung results. We believe that the positions and the Auger energies presented in this work will be helpful in identifying the resonances in future experiments.

ACKNOWLEDGMENT

I wish to thank Professor C. A. Nicolaides for his hospitality and discussions.

*Permanent address.

†Current address until the end of 1993.

- [1] C. F. Bunge, *Phys. Rev. A* **19**, 936 (1979); R. Jauregui and C. F. Bunge, *ibid.* **23**, 1618 (1981); W. Woznicki, M. Bylicki, B. Jaskolska, and J. Pipin (unpublished); K. T. Chung, *Phys. Rev. A* **29**, 682 (1984); K. T. Chung and B. F. Davis, *ibid.* **29**, 1871 (1984); **29**, 2586 (1984).
- [2] W. Woznicki, M. Bylicki, B. Jaskolska, and J. Pipin, *Chem. Phys. Lett.* **95**, 609 (1983).
- [3] S. Mannervik, *Phys. Scr.* **40**, 28 (1989).
- [4] M. Meyer *et al.*, *Phys. Rev. Lett.* **59**, 2963 (1987).
- [5] J. R. Peterson, M. J. Coggiola, and Y. K. Bae, *Phys. Rev. A* **23**, 59 (1981); *Phys. Rev. Lett.* **50**, 664 (1983).
- [6] C. A. Nicolaides and Y. Komninos, *Phys. Rev. A* **24**, 1103 (1981); *Chem. Phys. Lett.* **80**, 463 (1981).
- [7] B. F. Davis and K. T. Chung, *Phys. Rev. A* **41**, 5844 (1990).
- [8] M. Rødbro, R. Bruch, and P. Bisgaard, *J. Phys. B* **12**, 2413 (1979).
- [9] H. Feshbach, *Ann. Phys. (N.Y.)* **19**, 287 (1962); A. Temkin and A. K. Bhatia, in *Autoionization: Recent Developments and Applications*, edited by A. Temkin (Plenum, New York, 1985), pp. 1–34, 35–72.
- [10] M. Bylicki, *Phys. Rev. A* **40**, 1748 (1989).
- [11] M. Bylicki, *Phys. Rev. A* **39**, 3316 (1989).
- [12] A. Temkin and A. K. Bhatia, *Phys. Rev. A* **31**, 1259 (1985).
- [13] K. T. Chung, *Phys. Rev. A* **20**, 1743 (1979); K. T. Chung and B. F. Davis, in *Autoionization: Recent Developments and Applications* (Ref. [9]), p. 73.
- [14] K. T. Chung, *Phys. Rev. A* **41**, 4090 (1990); M. Bylicki, *ibid.* **41**, 4093 (1990); C. A. Nicolaides, *ibid.* **46**, 690 (1992); K. T. Chung, *ibid.* **46**, 694 (1992).
- [15] W. Thirring, *Quantum Mechanics of Atoms and Molecules*, Vol. 3 of *A Course of Mathematical Physics* (Springer, New York, 1981).
- [16] E. Träbert, P. H. Heckmann, J. Doerfert, and J. Grazow, *J. Phys. B* **25**, L353 (1992).
- [17] C. A. Nicolaides, *J. Phys. B* **25**, L91 (1992).
- [18] D. R. Beck and C. A. Nicolaides, *Chem. Phys. Lett.* **59**, 525 (1978).
- [19] K. Frankowski and C. L. Pekeris, *Phys. Rev.* **146**, 46 (1966).
- [20] Y. Accad, C. L. Pekeris, and B. Schiff, *Phys. Rev. A* **4**, 516 (1971).
- [21] O. Jitrik and C. F. Bunge, *Phys. Rev. A* **43**, 5804 (1991).