Feshbach-type projection method for multiply excited resonances

Mirosław Bylicki

Instytut Fizyki, Uniwersytet Mikołaja Kopernika, ul. Grudziądzka 5, PL-87-100 Toruń, Poland

(Received 7 March 1989)

A procedure for the Feshbach projection is presented. Although projection operators are not explicitly used within this procedure, it is completely equivalent to an explicit use of idempotent projectors, provided that both the target-state wave functions and the trial function of the entire system are of the configuration-interaction type. The Feshbach-projection-operator method is extended to the case of triply excited resonances (i.e., to an infinite number of open channels). Projectors are given explicitly for three-electron systems and for N-electron systems with the double-ionization threshold described by the (N-2)-electron one-determinant function. For configuration-interaction wave functions a procedure similar to that for doubly excited states is proposed.

I. INTRODUCTION

The projection-operator method for closed-channel resonances was introduced by Feshbach¹ in 1962. Since then it has been intensively applied in atomic physics.²⁻⁸ However, until recently, the rigorous implementation had been confined to two-electron systems² (i.e., to oneelectron targets) due to the following reasons. On the one hand, the original formulation of the method is not spin and symmetry adapted although all spin and spatial coordinates are implicitly included. On the other hand, it had seemed³ to be impossible to include in the projector all terms coming from exchange between incoming and orbital electrons. Therefore, a technique based on nonidempotent quasi-projection-operators, that do not include the exchange, was developed^{3,4} and successfully applied to three-electron systems.^{3,5} Finally, Temkin and Bhatia^{6,7} proposed a symmetry-adapted idempotent projector method for both elastic and inelastic scattering regions. So far, this method has been applied⁸ to the lowest resonant state of He⁻. An application of this method to the inelastic domain seems to be still complicated and has not yet been done. Even in the opinion of the authors of the method⁷ idempotent projectors are not yet likely to provide a useful calculational tool for the immediate future.

In Sec. II of this work a new practical procedure for realization of the Feshbach projection is proposed. This method does not involve target natural orbitals, in terms of which the projectors were expressed in both the Feshbach original formulation¹ and that of Temkin and Bhatia.⁶ Instead of making use of the projectors in explicit forms, the projection of a given function is to be found by solving a set of linear algebraic equations. Nevertheless, the procedure is equivalent to an explicit employment of idempotent operators, provided both the target-state wave functions and the trial function of the entire system are in configuration-expansion forms.

All the above-mentioned formulations of the projection method deal with a finite number of open channels. Each open channel is treated explicitly. This is impossible in a case of an infinite number of open channels, e.g., in a case of triply excited resonances. In Sec. III a method for triply excited resonances is proposed. It consists in Feshbach-type projection onto the space of open channels all of which are assumed to be connected with the ground state of the doubly ionized system. Explicit forms of P and Q projectors are derived for the three-electron system and for the *N*-electron system with double-ionization threshold described by one-determinant wave function. For a general case a procedure similar to that for doubly excited states is proposed. Some differences in the interpretation of the present formulation and the previous ones are discussed in Sec. IV.

II. FESHBACH PROJECTION FOR DOUBLY EXCITED RESONANCES

We are interested in resonant states of an N-electron system lying above the Mth state of the (N-1)-electron target. Let the lowest M energetically accessible target states be described by approximate wave functions ϕ_i , $i=1,\ldots,M$. Following Temkin and Bhatia^{4,6} we define open-channel wave functions in which those target states are coupled to the spin and orbital angular momentum of the Nth electron to form the considered total spin and orbital angular momentum of the entire system:

$$\psi_{v}(\mathbf{r}^{(N)}) = \sum_{m_{l},m_{s}} (L_{i} l M_{i} m_{l} | L M_{L}) (S_{i} \frac{1}{2} M_{s_{i}} m_{s} | S M_{s}) \times \phi_{i}(\mathbf{x}^{(N)}) Y_{lm_{l}}(\Omega_{N}) \chi_{\frac{1}{2}m_{s}}(N) , \qquad (1)$$

where, aside from the obvious notations for Clebsch-Gordan coefficients, $Y(\Omega_N)$ and $\chi(N)$ denote, respectively, the angular and spin functions of the Nth electron, $x^{(N)}$ indicates the absence of the totality of the coordinates describing the Nth electron, and $r^{(N)}$ denotes the absence of the radial coordinate of the Nth electron. The compound index ν consists of *i* and *l*. In general, there may be several values of *l* which can couple to form the considered *L* for a given *i*. On the other hand, it may also happen that it is impossible to form *L* and *S* for some values of *i*. Let *I* denote a set of indices $\nu = (i, l)$ such

<u>40</u> 1748

FESHBACH-TYPE PROJECTION METHOD FOR MULTIPLY ...

that $i \leq M$ and the considered L and S can be formed for i and l.

We define an open-channel space as the space of functions

$$\Phi = \mathcal{A} \sum_{v \in I} \psi_v(r^{(N)}) u_v(r_N) , \qquad (2)$$

where u_v is an arbitrary one-electron radial function. We assume that in the open-channel space we can find approximate wave functions of all the truly bound, resonant, and scattering states lying below the considered energy region as well as scattering states and shape resonances lying in the investigated domain. On the contrary, the approximate wave functions of Feshbach resonances are to be found in a closed-channel space, which is the orthogonal complement of the open-channel space to the *N*-electron antisymmetric-function space of a given symmetry.

The projection operators P and Q, projecting onto the open-channel and the closed-channel space, respectively, should satisfy the following conditions:

$$P\Psi = \mathcal{A} \sum_{v \in I} \psi_v(r^{(N)}) u_v(r_N) , \qquad (3)$$

$$P+Q=1 , \qquad (4)$$

$$P^2 = P , \qquad (5a)$$

$$Q^2 = Q$$
, (5b)

$$PQ=0, (5c)$$

$$P^{\dagger} = P$$
, (6a)

$$Q^{\dagger} = Q$$
 . (6b)

Equation (3) follows directly from the definition of the open-channel space, Eq. (2), and has a physical sense. All the remaining conditions are formal. The completeness condition, Eq. (4), determines that the idempotency, Eqs. (5a) and (5b), and orthogonality, Eq. (5c), conditions are dependent on one another. Similarly Eqs. (6) are mutually dependent. Thus, we have four independent conditions. The orthogonality (or idempotency) condition, Eq. (5c), means that, in our space of antisymmetrized wave functions for any Ψ and Ψ' , we have

$$\langle \Psi' | P Q \Psi \rangle = 0 . \tag{7}$$

We use Eqs. (6a) and (4) in Eq. (7) to obtain

$$\langle P\Psi' | (1-P)\Psi \rangle = 0 . \tag{8}$$

Keeping in mind that Ψ' is arbitrary, we see that the latter is equivalent to

for all pairs (μ, k) except those for which $\mathcal{A}\psi_{\mu}\varphi_{k}=0$. Equation (13) forms a set of linear algebraic equations for the coefficients $U_{\nu i}$ which is easy to solve by means of

any standard algorithm. When these coefficients are

found the $P\Psi$ and $Q\Psi$ projections are determined, ac-

cording to Eqs. (3) and (4), and they can be used in calcu-

lations of QHQ and/or the optical potential.

$$\langle \psi_{\mu}(r^{(N)})u(r_{N})|(1-P)\Psi\rangle = 0, \ \mu \in I$$
 (9)

Moreover, since u is arbitrary, Eq. (9) is equivalent to

$$\langle \psi_{\mu}(r^{(N)}) | (1-P)\Psi \rangle = 0, \ \mu \in I$$
, (10)

where the integration is over all the coordinates except r_N ; we are assuming throughout the convention that integration is performed over all coordinates appearing in bra parts of expressions. Inserting Eq. (3) into Eq. (10) gives

$$\langle \psi_{\mu}(\boldsymbol{r}^{(N)}) | \Psi \rangle = \sum_{\nu \in I} \langle \psi_{\mu}(\boldsymbol{r}^{(N)}) | \mathcal{A} \psi_{\nu}(\boldsymbol{r}^{(N)}) u_{\nu}(\boldsymbol{r}_{N}) \rangle , \quad (11)$$

which is a set of integral equations for functions u_{ν} , that are necessary for determination of $P\Psi$ for a given Ψ , Eq. (3).

A general expression for the operator P was obtained from Eqs. (3) and (11) by Temkin and Bhatia⁶ in a way analogous to that originally introduced by Feshbach.¹ This formal solution, although general and elegant, is difficult in practical application and usually demands some further approximations.

The other practical way for projection is to solve Eq. (11) for each given Ψ . The unknown functions u_{ν} can be found numerically for arbitrary forms of ϕ_i and Ψ . However, numerically solving Eq. (11) would be very expensive and therefore impractical. On the other hand, in a general case analytical solutions would be only approximate. However, if the wave functions ϕ_i $(i=1,\ldots,M)$ and trial function Ψ are of configuration-interaction type then exact analytical solutions for u_{ν} can be found. Now we direct our attention to this case.

Considering in Eq. (11) particular permutations, included in \mathcal{A} , it is easy to notice that all unknown functions u_v can be strictly expressed in terms of the radial orbitals which occur in target functions ϕ_i and in the function Ψ that is being projected. Therefore, we expect a solution as

$$u_{\mu}(\mathbf{r}_{N}) = \sum_{j \in J_{\mu}} U_{\mu j} \varphi_{j}(\mathbf{r}_{N}) , \qquad (12)$$

where φ_j are radial parts of orbitals used in ϕ_i , $i=1,\ldots,M$, and Ψ . As a matter of fact the summation is only over orbitals having the same angular symmetry as that connected with u_{μ} . This is emphasized by the subscript μ at J_{μ} , denoting a set of indices. By substituting expansion (12) into Eq. (11), multiplying them by each specific $\varphi_k(r_N)$, and integrating over r_N we have

$$\langle \psi_{\mu}(r^{(N)})\varphi_{k}(r_{N})|\Psi\rangle = \sum_{\nu \in I} \sum_{j \in J_{\nu}} \langle \psi_{\mu}(r^{(N)})\varphi_{k}(r_{N})|\mathcal{A}\psi_{\nu}(r^{(N)})\varphi_{j}(r_{N})\rangle U_{\nu j}$$

$$(13)$$

III. METHOD FOR TRIPLY EXCITED RESONANCES

In the case of triply excited resonances, lying above the double-ionization threshold, the number of open channels is infinite. Thus, the method described above is not applicable to this case. In the method proposed in this section all the open channels are handled at once.

1749

Let the ground state of doubly ionized system (doubleionization threshold) be described by the wave function $\phi(x^{(N-1,N)})$. Let us assume that all the (N-1)-electron thresholds lying below are associated with singly excited states of (N-1)-electron system, i.e., the (N-2)electron core is in the ϕ state. Now we can define an open-channel space as the space of antisymmetric Nelectron functions of a given symmetry with the (N-2)electron part described by ϕ . Thus, each function belonging to this space can be written as

$$\Phi = \mathcal{A} \sum_{v} \Lambda_{v} \phi(x^{(N-1,N)}) w_{v}(x_{N-1},x_{N}) , \qquad (14)$$

where $w_{\nu}(x_{N-1}, x_N)$ is an arbitrary two-electron function and Λ_{ν} stands for all the operations connected with the *LS* coupling. In general, there is a number of ways in which the required total symmetry can be obtained within the *LS* coupling. Therefore, the sum over ν appears in Eq. (14).

The projection operators P and Q, projecting, respectively, onto the open-channel space and its orthogonal complement, must fulfill the following conditions:

$$P\Psi = \mathcal{A} \sum_{\nu} \Lambda_{\nu} \phi(x^{(N-1,N)}) w_{\nu}(x_{N-1},x_N)$$
(15)

for an arbitrary antisymmetrized N-electron function Ψ , and

$$P + Q = 1, PQ = 0, P^{\dagger} = P$$
. (16)

These conditions are sufficient to find $P\Psi$ for a given Ψ .

In some cases even explicit P and Q operators can be derived from them.

A. Three-electron system

Explicit and rigorous forms for P and Q can be derived for a three-electron system. In this case Eq. (15) becomes

$$P\Psi = \mathcal{A}\phi(r_1)u(x_2, x_3, 1) , \qquad (17)$$

where $\phi(r_1)$ is the radial part of the one-electron function describing the double-ionization threshold (one-electron core) and $u(x_2, x_3, 1)$ is a function of two remaining electrons coupled to the spin and angular part of the core. The spin and angular coordinates of the core electron are denoted by 1. For convenience we assume $u(x_2, x_3, 1)$ antisymmetric in x_2 and x_3 , and the three-electron antisymmetrizer \mathcal{A} normalized by factor 1/2!. From Eqs. (16) and (17), in the same way as in Sec. II, we obtain

$$\langle \phi(\mathbf{r}_1) | \Psi \rangle = \langle \phi(\mathbf{r}_1) | \mathcal{A} \phi(\mathbf{r}_1) u(\mathbf{x}_2, \mathbf{x}_3, 1) \rangle , \qquad (18)$$

from which u can be found for a given Ψ .

Now we shall use this equation together with Eq. (17) for finding an explicit form of *P*. Equation (18) is equivalent to

$$\langle \phi(r_1) | \Psi \rangle = | u(x_2, x_3, 1) \rangle - | \phi(r_2) \rangle \langle \phi(r_1) | u(x_1, x_3, 2) \rangle - | \phi(r_3) \rangle \langle \phi(r_1) | u(x_2, x_1, 3) \rangle .$$
(19)

Multiplying the latter by $\phi(r_2)$ and integrating over r_2 we have

$$\langle \phi(r_1)\phi(r_2)|\Psi\rangle = \langle \phi(r_2)|u(x_2,x_3,1)\rangle - \langle \phi(r_1)|u(x_1,x_3,2)\rangle - |\phi(r_3)\rangle \langle \phi(r_1)\phi(r_2)|u(x_2,x_1,3)\rangle .$$
(20)

Similarly the analogous expressions for $\langle \phi(r_1)\phi(r_3)|\Psi\rangle$ and $\langle \phi(r_2)\phi(r_3)|\Psi\rangle$ can be obtained. Further, premultiplying Eq. (20) by $\phi(r_3)$ and integrating over r_3 we have

$$\langle \phi(r_1)\phi(r_2)\phi(r_3)|\Psi\rangle = \langle \phi(r_2)\phi(r_3)|u(x_2,x_3,1)\rangle - \langle \phi(r_1)\phi(r_3)|u(x_1,x_3,2)\rangle - \langle \phi(r_1)\phi(r_2)|u(x_2,x_1,3)\rangle .$$
(21)

We insert u from Eq. (19) into Eq. (17) to obtain

$$P\Psi = \mathcal{A}\left[\left|\phi(r_1)\right\rangle\left\langle\phi(r_1)\right|\Psi\right\rangle + \left|\phi(r_1)\phi(r_2)\right\rangle\left\langle\phi(r_1)\right|u(x_1, x_3, 2)\right\rangle + \left|\phi(r_1)\phi(r_3)\right\rangle\left\langle\phi(r_1)\right|u(x_2, x_1, 3)\right\rangle\right].$$
(22)

After performing antisymmetrization in Eq. (22) we use Eqs. (20) and (21) to obtain

$$P\Psi = (P_1 + P_2 + P_3 - P_1 P_2) - P_1 P_3 - P_2 P_3 + P_1 P_2 P_3)\Psi , \qquad (23)$$

where

$$\boldsymbol{P}_{i} \equiv |\boldsymbol{\phi}(\boldsymbol{r}_{i})\rangle \langle \boldsymbol{\phi}(\boldsymbol{r}_{i})| \quad .$$
(24)

Thus we have

$$P = P_1 + P_2 + P_3 - P_1 P_2 - P_1 P_3 - P_2 P_3 + P_1 P_2 P_3$$
(25)

and

$$Q \equiv 1 - P = \prod_{i=1}^{3} (1 - P_i) .$$
 (26)

One can see that these projectors are analogous to the Feshbach projectors for elastic-scattering domain of two-electron system.²

The operator Q has two interesting features. One is that due to the completely symmetric form Q commutes with the antisymmetrizer. The other is that the oneelectron operators $1-P_i$ are the same as the hole projectors used by Chung within his hole-projection technique.⁹ Thus in, the case of the three-electron system the projectors used by both methods are formally the same, although the Chung's derivation of his method was based on quite a different approach. The practical difference concerns the optimization of the $\phi(r)$ function. In the Feshbach-type projection method, proposed here, ϕ is the ground-state wave function of the hydrogenic ion while in Chung's method ϕ is the hole function optimized so to maximize the resonance energy. This notice completes considerations in Ref. 10, where the projection-operator method and hole-projection technique are compared.

B. One-determinant double-ionization threshold

Now we turn to the case of N > 3. Operators P and Q can be easily found for the ground state of doubly ionized system described by a one-determinant wave function $\phi(x^{(N-1,N)})$. Such an approximation is possible for a closed-shell (N-2)-electron ground state. For simplicity we confine our consideration to this case, although it is not the only one. Equation (15) takes the form

$$P\Psi = \mathcal{A}\phi(x^{(N-1,N)})u(x_{N-1},x_N) , \qquad (27)$$

where $u(x_{N-1},x_N)$ is an arbitrary but antisymmetric two-electron function of a proper symmetry; due to the ¹S symmetry of ϕ the total spin and angular momentum are the same as those of u. For convenience we assume that the N-electron antisymmetrizer \mathcal{A} is normalized by factor $1/\{2!(N-2)!\}$.

From Eqs. (16) and (27) we obtain

$$\langle \phi(x^{(N-1,N)}) | \Psi \rangle$$

= $\langle \phi(x^{(N-1,N)}) | \mathcal{A} \phi(x_1, \dots, x_{N-2}) u(x_{N-1}, x_N) \rangle$.
(28)

By considering all the permutations in the right-hand side of Eq. (28) we have

$$u(x_{N-1},x_N) = \langle \phi(x^{(N-1,N)}) | \Psi \rangle - {\binom{N-2}{2}} \langle \phi(x^{(N-1,N)}) | \phi(x_{N-1},x_N,x_3,\dots,x_{N-2}) u(x_1,x_2) \rangle + (N-2) \langle \phi(x^{(N-1,N)}) | \phi(x_N,x_2,\dots,x_{N-2}) u(x_{N-1},x_1) \rangle + (N-2) \langle \phi(x^{(N-1,N)}) | \phi(x_{N-1},x_2,\dots,x_{N-2}) u(x_1,x_N) \rangle .$$
(29)

Inserting the latter into Eq. (27) gives

$$P\Psi = \mathcal{A} \left| \phi(x^{(N-1,N)}) \right\rangle \left\langle \phi(x^{(N-1,N)}) \right| \Psi \right\rangle . \tag{30}$$

Thus the operator P is

$$P = \mathcal{A} \left| \phi(x^{(N-1,N)}) \right\rangle \left\langle \phi(x^{(N-1,N)}) \right| , \qquad (31)$$

which is completely analogous to that for onedeterminant target state in the case of doubly excited resonances in the elastic-scattering domain.¹

C. Configuration-interaction-type wave-functions case

If the form of the threshold function is more sophisticated, then an explicit form for P seems to be impossible to find. Therefore, a procedure analogous to that presented in Sec. II is proposed.

Let us assume that both the trial function Ψ and the ground-state wave function of the doubly ionized system are of the configuration-interaction type. Since it is impossible to separate the angular part from w_v in Eq. (15), we expand w_v in products of orbitals and then we separate the spin and angular parts. Thus, we can rewrite the Eq. (15) as

$$P\Psi = \mathcal{A} \sum_{\mu} \psi_{\mu}(r^{(N-1,N)})v_{\mu}(r_{N-1},r_N) , \qquad (32)$$

where

$$\psi_{\mu}(r^{(N-1,N)}) = \Lambda_{\mu}\phi(x^{(N-1,N)})Y_{\mu}(\Omega_{N-1})Y_{\mu}(\Omega_{N})\chi_{\mu}(N-1,N)$$
(33)

and v_{μ} is a product of two arbitrary one-electron radial functions. Because of the above-mentioned expansion of w_{ν} the index μ is quite different from ν and the sum over

 μ is infinite. However, in practice this sum can be truncated without a loss of strictness as can be seen later.

In the same way as before, we obtain a set of integral equations for v_{μ} :

$$\langle \psi_{\kappa}(r^{(N-1,N)}) | \Psi \rangle = \sum_{\mu} \langle \psi_{\kappa}(r^{(N-1,N)}) | \mathcal{A} \psi_{\mu}(r^{(N-1,N)}) v_{\mu}(r_{N-1},r_{N}) \rangle .$$
(34)

Since ϕ and Ψ are expressed in configuration-expansion forms then it follows from Eqs. (19) that v_{μ} are strictly expressible in pairs of radial orbitals appearing in Ψ and ϕ . Let φ_j , $j \in J_{\mu}$, denote such pairs. The subscript μ indicates that each v_{μ} is expressed in pairs of only those orbitals which correspond to the angular parts determined by μ . Only for a few values of μ we have $J_{\mu} \neq \emptyset$. For the remaining ones there is no pair of orbitals of the required symmetry among those occurring in ϕ and Ψ . Inserting the expansion

$$v_{\mu}(\mathbf{r}_{N-1},\mathbf{r}_{N}) = \sum_{j \in J_{\mu}} V_{\mu j} \mathcal{G}_{j}(\mathbf{r}_{N-1},\mathbf{r}_{N})$$
(35)

into Eqs. (19), premultiplying by each specific φ_k , and integrating over r_{N-1} and r_N gives

$$\langle \psi_{\kappa \mathscr{G}_{k}} | \Psi \rangle = \sum_{\mu} \sum_{j \in J_{\mu}} \langle \psi_{\kappa \mathscr{G}_{k}} | \mathcal{A} \psi_{\mu} \mathscr{G}_{j} \rangle V_{\mu j}$$
(36)

for all pairs (κ, k) for which $\mathcal{A}\psi_{\kappa \mathcal{G}k} \neq 0$. This is again a finite set of linear algebraic equations for the coefficients $V_{\mu j}$. If these coefficients are solved for, the $P\Psi$ and $Q\Psi$ projections are definitely determined and the QHQ calculations can be carried out.

IV. DISCUSSION

The basic property of the operator P, which has been required by Feshbach¹ and then by Temkin and Bhatia,⁶ is that P should preserve the asymptotic form of the exact resonant wave function; in other words, P should select out of the wave function the open-channel part. The projection procedure described above does have this property, although the asymptotic boundary condition for u was not postulated. When omitting the asymptotic requirement the actual interpretation of P is easily noticed: the projector P projects an arbitrary antisymmetric function onto the space of the lower-lying truly bound and resonance states as well as scattering states. This interpretation is especially important in the context of preventing a variational collapse in a QHQ calculation.

The interpretation of Eq. (11) is also found to be more general than in the previous papers.^{1,6} Equation (11) has been shown to follow from Eqs. (3)-(6) and to be equivalent to the requirement of idempotency of operators P and Q in the space of antisymmetric functions. Thus, once projection is performed according to Eq. (11), there is no need to worry about its idempotency. In the original Feshbach's paper¹ the equation corresponding to Eq. (11) was postulated as a condition sufficient for breaking up the wave function into two mutually orthogonal parts, one of which had the desired form (3). Moreover, in the paper of Temkin and Bhatia⁶ this equation was written for the exact resonance wave function only. That is why the property $P^2\Psi = P\Psi$ seemed to be obviously true only for the exact Ψ and a proof for an arbitrary antisymmetric function seemed to be necessary.^{6,7} However, one should realize that the form of P is influenced neither by the fact of satisfaction of the Schrödinger equation by Ψ nor by the asymptotic behavior of the u_{ν} functions. Hence, Eq. (2.9), or rather (B4) of Ref. 6, is in fact equivalent to our Eq. (11) and thus guarantees the idempotency of P and Q.

The projection procedure proposed in Sec. II is strictly equivalent to the use of the explicit projectors only for the configuration-interaction-type wave functions of both the doubly ionized and the entire system states. In practice this is not a very important limitation since for many-electron systems a configuration expansion is the mostly used ansatz for the wave function. Moreover, in the case of wave functions explicitly including interelectronic distances the procedure can be applied as an approximate method. The quality of this approximation will depend on the quality of the basis used in Eq. (12). As an example, let us consider a Hylleraas-type wave function for the two-electron target, which is the most advanced case in the approach of Temkin and Bhatia.⁶ Natural orbitals, in terms of which the projector *P* is constructed, are analytically approximated in a basis set.⁸ If we include this basis into expansion (12) and if we express the open-channel wave functions ψ_{μ} in Eqs. (13) in terms of given Hylleraas expansions then we obtain the approximation at least as good as in the explicit-projector approach.

It should be emphasized that although the projection procedure proposed here is less elegant it provides a simple computational algorithm that is essentially the same for resonances lying in the elastic scattering region as for those lying in the inelastic domain, and also for triply excited ones. Thus, all these states can be calculated by the same program. The method has been applied¹⁰ to the case of the 1s2s2p ²P° resonance of He⁻ within the generalized saddle-point method. This was the first application of the idempotent projection to the inelastic domain.

The projection method for triply excited resonances presented in Sec. III has never been formulated before. However, in the case of three-electron system the form of the projector Q has turned out to be the same as that used by Chung within his hole-projection technique.⁹ The same situation occurs in the case of doubly excited resonances in two-electron systems. Although the holeprojection technique, containing the mini-max idea for optimizing the energy of the autoionizing state, is not completely equivalent to the projection method, the results obtained by them for two-electron atoms are very close to each other.¹¹ I believe that the successful application of the hole-projection technique to triply excited resonances¹² in He⁻, Li, and Be⁺ justifies the reliability of the present approach.

ACKNOWLEDGMENTS

This work was carried out under the Polish Central Project for Fundamental Research No. CPBP 01.06.

- ¹H. Feshbach, Ann. Phys. **19**, 287 (1962).
- ²A. Temkin and A. K. Bhatia, in *Autoionization: Recent Developments and Applications*, edited by A. Temkin (Plenum, New York, 1985), pp. 1–34, and references therein.
- ³A. Temkin, A. K. Bhatia, and J. N. Bardsley, Phys. Rev. A 5, 1663 (1972).
- ⁴A. Temkin and A. K. Bhatia, Phys. Rev. A 18, 792 (1978).
- ⁵A. K. Bhatia and A. Temkin, Phys. Rev. A 13, 2322 (1976); A. K. Bhatia, *ibid.* 18, 2523 (1978); S. Wakid, A. K. Bhatia, and A. Temkin, *ibid.* 21, 496 (1980); 22, 1395 (1980); A. K. Bhatia and A. Temkin, *ibid.* 23, 3361 (1981).
- ⁶A. Temkin and A. K. Bhatia, Phys. Rev. A 31, 1259 (1985).

- ⁷A. Temkin and A. K. Bhatia, in *Autoionization: Recent Developments and Applications*, edited by A. Temkin (Plenum, New York, 1985), pp. 35–72.
- ⁸A. Berk, A. K. Bhatia, B. R. Junker, and A. Temkin, Phys. Rev. A **34**, 4591 (1986).
- ⁹K. T. Chung, Phys. Rev. A 20, 1743 (1979).
- ¹⁰M. Bylicki, Phys. Rev. A **39**, 3316 (1989).
- ¹¹K. T. Chung and B. F. Davis, in Autoionization: Recent Developments and Applications, edited by A. Temkin (Plenum, New York, 1985), pp. 73-102.
- ¹²K. T. Chung, Phys. Rev. A 22, 1341 (1980); 25, 1596 (1982); B.
 F. Davis and K. T. Chung, J. Phys. B 15, 3113 (1982).