PHYSICAL REVIEW A VOLUME 39, NUMBER 7 APRIL 1, 1989

Generalized saddle-point method for Feshbach resonances

Mirosław Bylicki
Instytut Fizyki, Uniwersytet Mikołaja Kopernika, ul. Grudziądzka 5, PL-87-100 Toruń, Poland
(Received 27 July 1988)

The mini-max principle is extended to work for the approximations to resonances in the square-integrable function space. The hole-projection (or saddle-point) technique for Feshbach resonances, introduced previously by Chung [Phys. Rev. A **20**, 1743 (1979)], is derived from the mini-max principle. Limits of applicability of the method are discussed and its generalization based on the Feshbach-type projector technique is given. The generalized method is applied to the case of the $1s2s2p\ ^2P^\circ$ resonance of He^-.

I. INTRODUCTION

The main obstacle in the application of variational methods to resonances in many-electron systems is the existence of an infinite space of states having the same symmetry as a resonance and lying below it. In general, the variational manifold should not contain these states. In order to remove them, the variational space is usually made orthogonal to some approximations of these states. Projection is the best method of orthogonalization. It is used in Feshbach-type projection-operator methods.[1-3] There exist also less accurate techniques such as the quasi-projection-operator method[4] and the one-particle projection-operator technique. In the latter one, introduced by Nicolaides,[5] the orthogonality of a trial function to the one-configurational approximations of lower-lying states is obtained by an appropriate orthogonalization of orbitals.

One-particle projectors of the same type have been used also by Chung[6-8] within his saddle-point, or hole-projection, technique. Chung's method originates from the physical intuition that vacancies should exist in the wave functions describing resonances. His papers are concerned with how to build these holes into a trial function and how to optimize them. The hole-projection is treated by him as a way of building-in the vacancy and not a method of orthogonalization. The presence of the vacancy is believed to stop a variational breakdown. That is why that method is reputed to be of a general nature.[6] However, there are many instances in which it does not work. Some of them are discussed in Sec. III of this paper.

A novelty introduced by Chung is that the energy of a resonance is maximized with respect to variations of the function describing a hole. An appropriate theorem was precisely proven for a one-particle system only.[6] One should realize that in this case the function describing a vacancy and total wave function of the system belong to the same one-electron space. Therefore the one-particle projector is a good projector operating in the Hilbert space of states of the entire system. Moreover, there are no autoionizing states in such a system. Hence the prescription for the energy of an excited state given by Chung's theorem[6] follows directly from the well-known mini-max principle.[9] The proof of Chung's theorem for a many-particle system[6] is unsatisfactory.

The main aim of this work is to properly interpret the saddle-point technique. Thus the prescription presented in Sec. III is strictly the same as that given by Chung. However, it is derived in a quite different way, starting from the mini-max principle.[9] This new derivation is simpler and more rigorous than that of Chung. Moreover, limitations of the method are clearly visible. It is indicated that the saddle-point technique should be generalized to avoid these limitations. Such a generalization consisting in the application of the Feshbach-type projectors within the mini-max principle scheme is presented in Sec. IV. Some numerical results obtained using this generalized method are given in Sec. V.

The mini-max principle is valid for a discrete spectrum only.[9] It is not applicable to resonance states because of continua of states which are not square integrable and lie below resonance levels. In Sec. II the mini-max principle is extended to work for the square-integrable approximations to resonances.

II. MINI-MAX PRINCIPLE FOR RESONANCES

We are interested in resonant states of an N-electron system autoionizing via Coulomb interaction between electrons. The Hamiltonian $\mathcal{H}$ is taken to be nonrelativistic and Hermitian. The domain of $\mathcal{H}$ can be divided into subspaces corresponding to distinct eigenvalues of operators commuting with $\mathcal{H}$, as, e.g., parity, total spin, and total orbital angular momentum. In this work we consider one such subspace. Furthermore, we want to describe the resonance by a square-integrable function and therefore instead of $\mathcal{H}$ we consider an operator $\underline{H}$ which is the representation of $\mathcal{H}$ in a space $\mathcal{D}$ of square-integrable N-electron functions of a given symmetry.

The best square-integrable approximations E_a and ψ_a to the energy and to the wave function of the resonance are a solution of the equation

$$\underline{H}\psi = E\psi \ . \tag{1}$$

The spectrum of $\underline{H}$ consists of eigenvalues corresponding to truly bound states and resonances and also to some scattering states, which are simulated in $\mathcal{D}$.

Let I_- and I_+ denote sets of indices of eigenvalues which are less than E_a and equal to or greater than E_a, respectively. It means that

$$E_i < E_a \quad \text{for } i \in I_- \tag{2a}$$

and

$$E_i \geq E_a \quad \text{for } i \in I_+ \ . \tag{2b}$$

We define two subspaces $\mathcal{D}_- \subset \mathcal{D}$ and $\mathcal{D}_+ \subset \mathcal{D}$ which are spanned by the sets of eigenfunctions $\{\psi_i\}_{i \in I_-}$ and $\{\psi_i\}_{i \in I_+}$, respectively. They are orthogonal complements of each other; in particular, $\mathcal{D}_+ = \mathcal{D}_-^{\perp}$.

For any normalized $\phi \in \mathcal{D}$ we have

$$\tilde{E} = \langle \phi | \underline{H} | \phi \rangle = E_a + \Delta E_- + \Delta E_+ \ , \tag{3}$$

where

$$\Delta E_- = \sum_{i \in I_-} (E_i - E_a) |\langle \psi_i | \phi \rangle|^2 < 0 \tag{3a}$$

and

$$\Delta E_+ = \sum_{i \in I_+} (E_i - E_a) |\langle \psi_i | \phi \rangle|^2 > 0 \ . \tag{3b}$$

If ϕ was orthogonal to $\mathcal{D}_-$, one could have $\Delta E_- = 0$ and

$$E_a = \inf_{\phi \in \mathcal{D}_-^{\perp}} \left\{ \frac{\langle \phi | \underline{H} | \phi \rangle}{\langle \phi | \phi \rangle} \right\} . \tag{4}$$

Unfortunately, one never knows the exact ψ_i, $i \in I_-$. Thus, in practice, ϕ can be orthogonalized only to approximate wave functions $\tilde{\psi}_i$, $i \in I_-$. Let $\tilde{\mathcal{D}}_-$ denote the space spanned by these functions. If $\tilde{\mathcal{D}}_- \neq \mathcal{D}_-$, then there exists $\phi \in \tilde{\mathcal{D}}_-^{\perp} \cap \mathcal{D}_-$ different from zero. For this ϕ we have $\tilde{E} = E_a + \Delta E_- < E_a$. The above consideration yields the following theorem:

$$E_a = \sup_{\tilde{\mathcal{D}}_- \subset \mathcal{D}} \inf_{\phi \in \tilde{\mathcal{D}}_-^{\perp}} \left\{ \frac{\langle \phi | \underline{H} | \phi \rangle}{\langle \phi | \phi \rangle} \right\} . \tag{5}$$

This means that E_a is equal to the maximal, as far as all the possible subspaces $\tilde{\mathcal{D}}_- \subset \mathcal{D}$ are considered, value of the minimum of the energy functional

$$K[\phi] = \frac{\langle \phi | \underline{H} | \phi \rangle}{\langle \phi | \phi \rangle} \ ,$$

provided that $\phi \in \tilde{\mathcal{D}}_-^{\perp}$.

The essential problem in practical implementation of the mini-max theorem is how to represent $\tilde{\mathcal{D}}_-$, which is infinite, and how to find its orthogonal complement $\tilde{\mathcal{D}}_-^{\perp}$. Sections III and IV are devoted to these questions.

III. HOLE-PROJECTION METHOD

In this section the prescription introduced originally by Chung[6] is derived from the mini-max principle.

The crucial point of the hole-projection method is the orthogonalization via the projection of a hole, in other words, via building a vacancy into the trial function. In order to perform the hole projection it is enough to consider an electronic configuration only. That is why in this section we neglect the symmetry of total wave function. It is assumed that antisymmetrization and coupling of spin and orbital angular momenta are to be performed after the hole projection.

Let F^N be a Hartree-type product of N abstract orbitals which are ordered with respect to the principal and orbital quantum numbers. Such a product corresponds to an electronic configuration of an N-electron system. In this paper the configuration is identified with the corresponding Hartree product.

A. Model

Let the autoionizing state that we want to investigate be a Feshbach resonance connected with the first excited state of the $(N-1)$-electron target. Thus the configuration corresponding to it can be written as

$$F_a^N = F_1^{N-1} \varphi_a \ , \tag{6}$$

where φ_a is an orbital and F_1^{N-1} is the configuration describing the first excited target state. Then let us suppose that all the states lying below our resonance are associated with the ground state of the target and their configurations can be written in the form

$$F_i^N = F_0^{N-1} \varphi_i, \quad i \in I_- \ , \tag{7}$$

where the configuration F_0^{N-1} describes the ground state of the target. Moreover, we assume that configurations F_0^{N-1} and F_1^{N-1} differ by at least one orbital, e.g.,

$$F_0^{N-1} = F_0^{N-2} \varphi_0 \tag{8}$$

and

$$F_1^{N-1} = F_0^{N-2} \varphi_1 \ , \tag{9}$$

where $\varphi_1 \neq \varphi_0$. Hence, if φ_0 occurs p times in F_0^{N-2}, then it occurs at least $p+1$ times in configurations F_i^N $(i \in I_-)$, whereas in F_a^N it is occupied by p electrons only. In this sense the φ_0 hole is present in F_a^N.

B. Derivation of the method

Let us express the above considerations in terms of the mini-max theorem. We approximate $\mathcal{D}_-$ by a space $\tilde{\mathcal{D}}_-$ spanned by all the configurations in which φ_0 is occupied by at least $p+1$ electrons. Then $\tilde{\mathcal{D}}_-^{\perp}$ includes all the configurations in which no more than p electrons occupy orbitals nonorthogonal to φ_0. This means that in any configuration belonging to $\tilde{\mathcal{D}}_-$ at most p orbitals of the same symmetry as φ_0 may remain arbitrary while all the others have to be orthogonalized to φ_0. This orthogonalization is called the hole projection.

Let us note that $\tilde{\mathcal{D}}_-^{\perp}$ is orthogonal to the approximate scattering states in which the target is in the F_0^{N-1} configuration. The scattering states lie below as well as above the considered resonance. Hence the $\tilde{\mathcal{D}}_-$ space is too large in the context of the mini-max principle. Since there is no simple way to distinguish between the scattering states lying below the resonance and those lying

above, we can only believe that the influence of the latter ones is negligible.

One can vary $\tilde{\mathcal{D}}_-$, changing the hole function φ_0. Let φ_0 be parametrized by a set of parameters q. Then a trial function $\phi \in \tilde{\mathcal{D}}^{\perp}_-$ depends on its own parameters α and, due to the hole projection, also on q. In order to carry out the prescription given by the mini-max theorem, Eq. (5), one should minimize the energy expectation value,

$$\tilde{E} = \langle \phi | \underline{H} | \phi \rangle / \langle \phi | \phi \rangle \ ,$$

with respect to parameters α and simultaneously maximize it with respect to q.

This prescription is valid for the lowest Feshbach resonance lying in the elastic scattering region. Approximate energies of resonances lying just above the lowest one can be obtained by means of the Ritz method (applied to the linear parameters in α) as consecutive roots of the corresponding secular equation. Solutions obtained in this way are orthogonal to one another. Moreover, since the basis functions belong to $\tilde{\mathcal{D}}^{\perp}_-$, all of them are orthogonal to configurations describing the lower-lying states. Thus the consecutive roots given by the Ritz method approximate energies of the corresponding resonances. There are at least two possible ways of optimization with respect to q: the maximization of each root individually or the maximization of the lowest root only.

C. Resonances in inelastic scattering regions

Now let us deal with a case of autoionizing levels lying in the inelastic scattering region. As an example we consider resonances lying between the two lowest excited levels of the target. Let us assume that the electronic configurations describing these states are of the form

$$F^N = F_2^{N-1} \varphi \ , \tag{10}$$

where the core F_2^{N-1} is a configuration corresponding to the second excited state of the target. Suppose that

$$F_2^{N-1} = F_0^{N-2} \varphi_2 \tag{11}$$

and that it is different from both F_0^{N-1} and F_1^{N-1} defined by Eqs. (8) and (9), i.e., that $\varphi_2 \neq \varphi_0$ and $\varphi_2 \neq \varphi_1$ (the condition $\varphi_1 \neq \varphi_0$ is not necessary now). Thus one can say that the φ_0 and φ_1 vacancies are present in F^N. The vacancies should be built into the trial function in the same way as before. Since φ_0 and φ_1 describe the space of states lying below the investigated resonances, the expectation value of the energy should be maximized with respect to parameters in these orbitals. When considering higher autoionizing states one should remember that they must be assigned to configurations containing more holes than the ones associated with the lower-lying states.

The hole-projection technique can treat also more than doubly excited resonances,[7] i.e., the ones lying above the multiple ionization thresholds. Although the number of open channels is then infinite, the number of vacancies needed to orthogonalize the trial function to all of them may be quite small. That is because the target states related to our resonances are one time more excited than the ones corresponding to the open channels. Therefore the vacancies appear in deeper shells and are filled in all, or almost all, the open channels. For example, a triply excited resonance of the lithium atom lying just above the $1s$ state of Li^{2+} can be approximated by the configuration $2s n_1 l_1 n_2 l_2$, whereas the configurations corresponding to states lying below this threshold are $1s n_1' l_1' n_2' l_2'$. Therefore, in order to orthogonalize the trial function to the lower-lying states, we should build the $1s$ vacancy into it, that is, all the orbitals in the trial function should be orthogonal to $1s$.

D. Discussion

In real systems, especially in ionized ones, the series such as those defined in Eqs. (6) and (7) are not energetically separated and disturb each other. This means that there may exist some doubly excited states of the type (6) which lie below the ionization threshold or some resonances associated with the second excited target state which lie below the first excited level of the target, etc. However, the number of such states is usually small and therefore the higher roots obtained by the Ritz method correspond to resonances in the region under consideration.

Furthermore, the classification of the states in terms of configurations as given by Eqs. (6) and (7) is approximate. Feshbach resonances are often degenerated, that is, they are associated with several closed channels.[7] The hole-projection technique holds true in this case, provided that the appropriate vacancies are present in all the configurations which are necessary to describe the resonance.

The total symmetry of the wave function was not taken into account when deriving the hole-projection technique. However, it may happen that some terms in the configurational expansion are orthogonal to some open channels just because of the spin- and/or orbital-angular-momenta coupling scheme (see the example of He^- discussed below). For those terms the hole-projection procedure can be restricted to a lesser number of vacancies or relaxed.

There are many systems in which different target states connected with a series of resonances and a series of lower-lying states are related to the same configuration, i.e., there is no hole to distinguish between them. For example, the C-like target[10] has the ground state ^1S and two succeeding excited states ^1D and ^3P which can be derived from the same $1s^2 2s^2 2p^2$ configuration. Every one of them can be a parent state for a series of $^2P^\circ$ states of the seven-electron system, and no hole can be defined to distinguish between these series.

A similar, but even more misleading situation is found in He^-. The first and the second excited states of He (target) are $1s2s\ ^3S$ and $1s2s\ ^1S$. The resonance $1s2s2p\ ^2P^\circ$ is found in the region between them.[7,11-19] One may believe that the $1s$ vacancy, when built into the trial function, is sufficient to stop the unwelcome lowering of the $^2P^\circ$ energy. However, that vacancy is sufficient to orthogonalize the trial function to the $1s^2 np$ series only but not to the $1s2s(^3S)np\ ^2P^\circ$ one. It may seem that it is no matter since in He^- both the $1s^2 np$ and $1s2s(^3S)np\ ^2P^\circ$

series do not really exist. But then there are scattering states in He^- which can be imitated by these configurations and therefore they cause a variational breakdown. This fact may be seen in Fig. 1 and Fig. 2 of Ref. 7, though it was not the intention of the authors. The energy of the $^2P^\circ$ resonance is plotted there as a function of one of the nonlinear parameters used by Chung and Davis in their calculations.[7] Those figures correspond to the basis of singlet– and triplet–intermediate-coupling terms, respectively. All the curves in Fig. 1 lie above the experimental position of the $^2P^\circ$ resonance, whereas the curves in Fig. 2 lie below that level. That is just because all the terms with singlet intermediate coupling are orthogonal to $1s2s\ ^3S$, whereas some of their counterparts with triplet intermediate coupling are not.[20] It is obvious, because of the MacDonald[21] theorem, that a superposition of these two basis sets should give results lower than those in Fig. 2 of Ref. 7. Hence the absence of terms with triplet intermediate coupling in the final calculations by Chung[11] and Chung and Davis[7] had a vital importance; the pure hole-projection technique would be useless in this case. Chung did not notice this fact[22] because in his formulation of the saddle-point technique the hole projection is regarded as sufficient by itself to prevent a variational breakdown, and the vacancies are defined in relation to the capacity of the inner subshells rather than in relation to the occupancy of orbitals in the states lying below the investigated energy region.

IV. GENERALIZED SADDLE-POINT METHOD

The above discussion shows that a generalization of the saddle-point method is needed. The generalization overcoming main difficulties which appear in the hole-projection technique is presented in this section.

Let us consider resonances lying in the elastic scattering region. All the states lying below are assumed to be associated with the ground state of the $(N-1)$-electron target. Therefore we approximate $\mathcal{D}_-$ by $\tilde{\mathcal{D}}_-$ spanned by functions of the form

$$\tilde{\psi}^N(x_1,\ldots,x_N;q)=\mathcal{A}\Lambda[\phi_0^{N-1}(x_1,\ldots,x_{N-1};q)\varphi(x_N)]\ , \tag{12}$$

where x_i is a set of spin and spatial coordinates of the ith electron, $\mathcal{A}$ is the antisymmetrizer, Λ denotes a coupling operator producing functions of proper spatial and spin symmetries, φ is an arbitrary but square-integrable spin-orbital, and

$$\phi_0^{N-1}(x_1,\ldots,x_{N-1};q)$$

is any approximate wave function of the target ground state, and q is a set of parameters. When the hole-projection technique was being outlined in Sec. III, the assumption on the structure of $\tilde{\mathcal{D}}_-$ was similar but the description of the target ground state was very specific. Now ϕ_0^{N-1} is arbitrary. Moreover, its symmetry is taken into account in Eq. (12), so it will affect the orthogonality constraints.

We can build the projection operator P projecting onto $\tilde{\mathcal{D}}_-$, defined in Eq. (12), according to the Feshbach theory[1] in the spin and symmetry adapted form proposed by Temkin and Bhatia.[2] The operator $Q=I-P$ is the projector onto $\tilde{\mathcal{D}}_-^{\perp}$. The mini-max principle demands that a trial function should belong to $\tilde{\mathcal{D}}_-^{\perp}$. In practical calculations we can take an arbitrary N-electron trial function ϕ dependent on parameters α and then project it onto $\tilde{\mathcal{D}}_-^{\perp}$. Since projectors P and Q are dependent on q, $Q\phi$ depends on q too. The mini-max theorem can be rewritten in the form

$$E_a \simeq \sup_q \inf_\alpha \left\{ \frac{\langle Q(q)\phi(\alpha)|\underline{H}|Q(q)\phi(\alpha)\rangle}{\langle Q(q)\phi(\alpha)|Q(q)\phi(\alpha)\rangle} \right\}, \tag{13}$$

i.e., the approximation to the energy E_a (the best in the square-integrable approximation) of the lowest Feshbach resonance is to be found as the saddle point of the energy expectation value, the minimum with respect to α and simultaneously the maximum with respect to q, provided the trial function is projected onto $\tilde{\mathcal{D}}_-^{\perp}$.

Approximate energies of higher Feshbach resonances lying in the elastic scattering region can be obtained as consecutive roots by the Ritz method, as in the hole-projection technique. In order to get energies of resonances lying in the inelastic scattering regions one should use projectors proposed by Temkin and Bhatia[2] and maximize the energies with respect to variations of all the target states which are energetically open.

The relationship of this method to the Feshbach projection-operator method is like the relationship of Chung's hole-projection technique to the hole-projection proposed by Nicolaides.[5] Projection operators are strictly the same as those by Temkin and Bhatia[2] but the way of optimization of the target open state ϕ_0 is different. In the Feshbach method ϕ_0^{N-1} should be the best possible approximation to the ground state of the *isolated* target. On the contrary, in the generalized saddle-point method $\phi_0^{N-1}(q)$ is the $(N-1)$-electron-*core* function. Due to the maximization of the resonance energy with respect to q, ϕ^{N-1} is averaged, in a way, all over $\mathcal{D}_-$. This extra maximization makes the method more expensive than the Feshbach projector method. Nevertheless, if just the square-integrable approximation is considered, then this manner of optimization of ϕ_0^{N-1} seems to be more plausible. It seems to be reasonable to take $\phi_0^{N-1}(q)$ in a relatively simple form and to maximize the resonance energy with respect to q instead of using an elaborate ϕ_0^{N-1} optimized for the isolated target.

V. CALCULATION

The generalized saddle-point method has been applied to the $1s2s2p\ ^2P^\circ$ resonance of He^-. That particular case has been chosen just because, in principle, the hole-projection technique is here not applicable (see discussion above).

Two target states are energetically accessible in that case. These are the ground state ^1S and the first excited state $2\ ^3S$ of He. Their approximate wave functions are chosen in the forms

$$\phi_0^{N-1}(x_1,x_2;q_0)=C_0 e^{-q_0(r_1+r_2)}\chi_{00} \tag{14a}$$

and

$$\phi_1^{N-1}(x_1,x_2;q_1,q_2)=C_1(\,r_2e^{-(q_1r_1+q_2r_2)} - r_1e^{-(q_2r_1+q_1r_2)})\chi_{1m}\ , \quad (14b)$$

where C_0 and C_1 are normalization factors; r_1 and r_2 are the radial coordinates of electrons; χ_{sm} is a two-electron spin function of the total spin s and the spin component m. The space $\tilde{\mathcal{D}}_-$ consists of linear combinations of functions

$$\psi=\mathcal{A}\phi_0^{N-1}(x_1,x_2;q_0)\varphi(x_3) \quad (15a)$$

and

$$\psi=\mathcal{A}\sum_m \phi_1^{N-1}(x_1,x_2;q_1q_2)\varphi(x_3)\ , \quad (15b)$$

where φ represents all possible spin-orbitals p; the summation over m is due to the spin coupling of the third electron.

The three-electron trial function ϕ is taken in a configuration expansion form using the Slater-type orbitals. To project ϕ onto $\tilde{\mathcal{D}}^{\perp}_-$ one could use projectors derived by Temkin and Bhatia for many open channels.[2] However, the author has used his own matrix version of the Feshbach projection-operator method.[3] It is completely equivalent to the use of projectors by Temkin and Bhatia, provided that configuration expansions are used for both the target-state wave functions and the trial function of the entire system. The advantage of this method is that the computational algorithm is much simpler.

In the actual calculation eleven angular partial waves have been used, including both singlet and triplet intermediate couplings. They are displayed in Table I together with their contributions to the $^2P^\circ$ energy. Nonlinear parameters have been taken from the Ref. 11, where they were optimized by Chung for the partial waves with singlet intermediate coupling. The triplet–intermediate-coupling terms, included in this work, have the same nonlinear parameters as their singlet–intermediate-coupling counterparts. Nevertheless, their contributions to the $^2P^\circ$ resonance energy are not at all negligible.

The $[(s,s)^3S,p]$ partial wave is especially noteworthy. It is not orthogonal to the $2\,^3S$ He state. When projected onto $\mathcal{D}^{\perp}_-$ it lowers the energy by 0.000 099 a.u. However, if it is left nonorthogonal to ϕ_1^{N-1} it causes a variational breakdown (confirmed also in an explicit numerical experiment performed by the author—the resulting energy was near the $2\,^3S$ threshold). All the remaining triplet–intermediate-coupling partial waves are orthogonal to ϕ_1^{N-1}, Eq. (14b), and could be included in a hole-projection-technique calculation as well.

As we can see the convergence of the basis set is slower than the convergence obtained by Chung.[11] That is because the radial term selection process has been performed not as carefully as Chung had done.[11]

The q parameters have been optimized keeping nonlinear parameters for all the partial waves unchanged. As a start for searching for the $^2P^\circ$ energy maximum the values $q_0=1.6875$, $q_1=1.995$, and $q_2=0.565$ have been used. They correspond to the minima of the target-state energies at $-2.847\,656$ and $-2.172\,500$ a.u. for $1s^2\,^1S$ and $1s2s\,^3S$, respectively. The total $^2P^\circ$ energy corresponding to them is $-2.151\,395$ a.u., that is, 20.472 eV above the helium ground state. It is included in Table II as a result obtained by the projection-operator method. The optimized values of q are $q_0=1.52$, $q_1=1.83$, and $q_2=0.27$ (q_0 obtained by Chung[11] is 1.5). These values were used to obtain all the results presented in Table I.

The final eleven–partial-wave result, $-2.149\,151$ a.u., lies at 20.533 eV above the helium ground state. It is compared in Table II with other theoretical and experimental results. One can see that the results obtained by methods using closed-channel wave functions (first five in Table II) are close to one another. They differ essentially from the remaining theoretical results, in which the in-

TABLE I. Calculation of the energy of the $1s2s2p\ ^2P^\circ$ resonance of He^-. ΔE is the contribution to the binding energy due to the given partial wave.

Partial wave	Number of terms	Nonlinear parameters			$-\Delta E$ (a.u.)
$[(s,s)^1S,p]$	24	2.0	0.54	0.345	2.141 230
$[(s,p)^1P,d]$	4	2.0	0.515	0.42	0.006 211
$[(p,p)^1S,p]$	8	2.0	1.6	0.24	0.000 773
$[(s,d)^3D,p]$	5	2.0	0.44	0.77	0.000 439
$[(s,p)^3P,d]$	4	2.0	0.515	0.42	0.000 187
$[(s,s)^1S,p]$	9	2.0	1.6	0.24	0.000 117
$[(s,s)^3S,p]$	15	2.0	0.54	0.345	0.000 099
$[(p,d)^1P,d]$	4	1.6	1.84	0.37	0.000 037
$[(s,d)^1D,f]$	2	2.0	0.69	0.87	0.000 029
$[(d,d)^1S,p]$	1	2.9	3.0	0.25	0.000 018
$[(s,d)^3D,f]$	2	2.0	0.69	0.87	0.000 011
Total	78				2.149 151

TABLE II. Energy of the He^- $1s2s2p\ ^2P^\circ$ resonance relative to the He ground-state level.

	E (eV)	Method
Theory	20.536	hole-projection, Ref. 11
	20.495	quasi-projection-operator,[a] Ref. 11
	20.525	quasi-projection-operator,[a] Ref. 12
	20.533[b]	generalized saddle-point, this work
	20.472[b]	projection-operator, this work
	20.17	matrix variation, Ref. 14
	20.19	R-matrix, Ref. 15
	20.33	complex stabilization, Ref. 16
	20.26	resonance scattering theory, Ref. 13
Experiment	20.27 ∓ 0.01	Ref. 17
	20.40 ∓ 0.03	Ref. 18
	20.5	Ref. 19

[a]In my opinion these results should be referred to as being obtained by the projection-operator method. There is no difference between projectors and quasiprojectors when the target function is one-determinant.

[b]The target-ground-state energy, $-2.903\,724$, is taken from Ref. 23 (1 a.u. $=27.211\,652$ eV).

teraction with the open-channel continuum is taken into account. The magnitude of the $^2P^\circ$ width[17] shows that the coupling with the continuum is rather strong and a shift in the resonance position caused by it should be quite large. The existing experimental data differ between one another. They lie in the range from 20.27 to 20.5 eV. Therefore it is rather difficult to state definitely which theoretical result is the best one.

VI. SUMMARY

The original formulation of the saddle-point technique by Chung[6] is based on the assumption that Feshbach resonances can be considered as quantum states with well-defined inner-shell vacancies. The vacancies are defined considering an electronic configuration (or several-configuration mixture) corresponding to the resonance under consideration. In Chung's opinion the building in a vacancy or vacancies is itself enough to prevent a variational breakdown. However, it may happen that the same vacancies occur in states lying below the considered one. In such a case these states will arise as results of the hole-projection calculation instead of the expected ones. In this sense they are spurious. The misunderstanding comes from the improper way of deriving the method by Chung.[6]

In this work the hole-projection method has been rederived starting from the mini-max principle extended to be valid for square-integrable approximations to resonances. In this context the hole projection is a method of orthogonalization of a trial function to the space of lower-lying states of the same symmetry. This orthogonalization plays a crucial role in preventing a variational collapse. When the "well-defined" vacancies are not sufficient to distinguish between the resonances under consideration and all the lower-lying states of the same symmetry, then some additional constraints are needed, e.g., omitting the triplet–intermediate-coupling terms in the case of the $1s2s2p\ ^2P^\circ$ resonance in He^-. That is why each case that the hole-projection technique is to be applied to should be carefully analyzed in order to decide whether some additional constraints are required or not.

Difficulties appearing in the hole-projection technique do not occur in the generalized saddle-point method which has been also derived in this work from the mini-max principle. Feshbach-type projectors are used in it in order to orthogonalize the variational manifold to the open channels. The resonance energy is maximized with respect to variations of the wave functions of the target states which are energetically accessible. This method completes the environment in which the hole-projection technique may be interpreted. It confirms and explains Temkin's opinion[24] that the hole-projection technique can be considered in the category of quasiprojectors.

The generalized saddle-point method has been applied to find the energy of the $1s2s2p\ ^2P^\circ$ resonance of He^-. The result is in accordance with the results of calculations by Chung[11] and Bhatia and Temkin[12] in which square-integrable wave functions have been used. The contributions of triplet–intermediate-coupling terms, which had not been included in the above-mentioned calculations, have been found to be not negligible.

ACKNOWLEDGMENT

This work was carried out under the Polish Central Project for Fundamental Research CPBP 01.06.

[1]H. Feshbach, Ann. Phys. (N.Y.) **19**, 287 (1962).

[2]A. Temkin and A. K. Bhatia, Phys. Rev. A **31**, 1259 (1985); in *Autoionization: Recent Developments and Applications*, edited by A. Temkin (Plenum, New York, 1985), p. 35.

[3]M. Bylicki (unpublished).

[4]A. Temkin, A. K. Bhatia and J. N. Bardsley, Phys. Rev. A **7**, 1663 (1972); A. Temkin and A. K. Bhatia, *ibid.* **18**, 792 (1978).

[5]C. A. Nicolaides, Phys. Rev. A **6**, 2078 (1972).

[6]K. T. Chung, Phys. Rev. A **20**, 1743 (1979).
[7]K. T. Chung and B. F. Davis, in *Autoionization: Recent Developments and Applications,* edited by A. Temkin (Plenum, New York, 1985), p. 73.
[8]K. T. Chung, Chin. J. Phys. **25**, 215 (1987).
[9]W. Thirring, *Quantum Mechanics of Atoms and Molecules,* Vol. 3 of *A Course of Mathematical Physics* (Springer, New York, 1981).
[10]S. Bashkin and J. O. Stoner, Jr., *Atomic Energy Levels and Grotrian Diagrams* (North-Holland, Amsterdam, 1975).
[11]K. T. Chung, Phys. Rev. A **23**, 1079 (1981).
[12]A. K. Bhatia and A. Temkin, Phys. Rev. A **23**, 3361 (1981).
[13]Y. Komninos, G. Aspromalis, and C. A. Nicolaides, Phys. Rev. A **27**, 1865 (1983).
[14]R. S. Oberoi and R. K. Nesbet, Phys. Rev. A **8**, 2969 (1973).
[15]W. C. Fon, K. A. Berrington, P. G. Burke, and A. E. Kingston, J. Phys. B **11**, 325 (1978).
[16]B. R. Junker, J. Phys. B **15**, 4495 (1982).
[17]J. N. H. Brunt, G. C. King, and F. H. Read, J. Phys. B **10**, 433 (1977).
[18]F. Pichou *et al.*, J. Phys. B **9**, 933 (1976).
[19]J. M. Phillips and S. F. Wong, Phys. Rev. A **23**, 3324 (1981).
[20]Bhatia and Temkin used this fact purposely in their calculations of the $^2P^\circ$ resonance in He^-; see Ref. 12.
[21]J. K. L. MacDonald, Phys. Rev. **43**, 830 (1933).
[22]The reason for which Chung has omitted triplet–intermediate-coupling terms was that in his opinion their contribution in the lowering of the total $^2P^\circ$ energy is negligible.
[23]C. L. Pekeris, Phys. Rev. **136**, 143 (1962); **136**, 1470 (1962).
[24]See the Preface in *Autoionization: Recent Developments and Applications,* edited by A. Temkin (Plenum, New York, 1985).