Reply to "Comment on 'Generalized saddle-point method for Feshbach resonances'"

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It is argued that the saddle-point method developed by Chung [Phys. Rev. A **20**, 1743 (1979)] may be considered in the category of orthogonalization to the open-channel space, and that the generalization of the method introduced by Bylicki offers a precise prescription for implementation of the original formulation by Chung.

The saddle-point, or hole-projection, technique introduced by Chung[1] is a very efficient method. A list of really important and accurate results obtained by this method is given by Chung in the previous Comment.[2] At the same time this method is very simple in practical application.

Although Chung claimed in the Comment[2] that he did not derive the method, I regard his first paper, Ref. 1, as containing a derivation of it. I have found this derivation incomplete. The theorem formulated and proved by Chung[1] for a one-particle system has no practical meaning. There are no resonances in such a system. Moreover, the prescription for the energy of an excited state given by Chung follows directly from the well-known mini-max principle.[3] The first statement of Sec. IV in Ref. 1 suggests that this section contains a generalization of a one-particle case to a many-body system. I have found considerations presented in this section rather complicated and obscure. In particular, conditions sufficient for preventing a variational breakdown were not precisely stated there.

In my paper,[4] which is being criticized[2] by Chung, I rederived the hole-projection method starting from the mini-max principle. The hole-projection procedure turned out to be a method of orthogonalization of a trial function to some approximation of the space of lower-lying states of the same symmetry as that of a considered resonance. This is in disagreement with the original formulation of the saddle-point method,[1] although this is in accordance with the interpretation by Nicolaides,[5] who defined the hole-projection operators for the first time. Chung has stated[1] that a vacancy is built directly into the trial function *instead* of making it orthogonal to the open channels. He admitted in the Comment[2] that he had checked the orthogonality in a few cases and it was achieved to an *amazing* degree. This is not amazing at all. In this Comment I shall show that the *orthogonality* of the trial function to the open channels is the *essence* of the hole-projection technique; this is why the method works.

Chung has not formulated a unique prescription for determining vacancies in the "inner-shell-vacancy picture." However, the examples given by him suggest that the vacancies are defined by comparing the electronic configuration (or several configuration mixtures) corresponding to a given resonance with maximal possible occupancies of the inner subshells. Let us notice that if such vacancies are built into the trial function, but they are filled in all the open-channel states lying below the resonance, then the orthogonality to the open channels is achieved. Nevertheless, it may happen that the considered resonance, and some lower-lying open-channel states, are not distinguishable within the "inner-shell-vacancy picture."

This is the case of the $1s2s(^1S)2p\ ^2P^\circ$ resonance in He^-. The only vacancy which can be seen in the "inner-shell-vacancy picture" of this state is the $1s$ hole. But the same vacancy is present in $1s2s(^3S)np$ functions which represent the open channel. Each partial wave one uses in the trial function should be orthogonal to this open channel. The only nonorthogonal one is the $[(s,s)^3S,p]$ partial wave. It is simply omitted in Chung's calculation together with other triplet-intermediate-coupling terms. Although, in the Comment,[2] Chung gives some reasons for omitting the $[(s,s)^3S,p]$ partial wave in the case of He^- $1s2s2p$ resonance calculation, the only reason given in the original paper, Ref. 6, was that "the terms with triplet-intermediate coupling contribute little to the lowering of the $^2P^\circ$ total energy." In the Comment[2] Chung stated that "one must build the proper vacancy such that the open channel is removed," and he proposed to include the $[p(s,s)^3S]$ partial wave orthogonalizing both s orbitals to the $1s$ "vacancy" orbital. But are these two $1s$ vacancies natural in the "inner-shell-vacancy picture?" Building these *auxiliary* holes into the $[p,(s,s)^3S]$ partial wave, one makes it orthogonal to the $1s2s(^3S)np$ open channel. (This is the actual meaning of "removing the open channel.") It works. But in my opinion this prescription did not follow from the original formulation.

It should be emphasized that the $^2P^\circ$ resonance of He^- is just an example, but not the only one in which the "inner-shell-vacancy picture" is not enough to distinguish between the resonance and some lower-lying open-channel states. The same situation is in the case of $1s2s(^1S)nd$, $n=3,4,5$, resonances in Li. This time the omission of the $[(s,s)^3S,d]$ partial wave in the trial function was left by Chung[7] without any explanation. In Ref. 4, I also gave an example concerning resonances in the seven-electron system which cannot be treated by the hole-projection technique.

Chung claimed[2] that he had never tried to define a P space for orthogonalization. That is true, he has never

done it consciously. Nevertheless, when building the vacancy into a trial function, he actually orthogonalizes it to a specific approximation of the P space. Let us look at this approximation in the case of $1s2s2p\ ^2P^\circ$ resonance in He^-. When the $1s_q$ vacancy is built into a trial function, then it is made orthogonal to $1s_q^2np$ configurations, which represent the first open channel. Note that the description of target ground state, $1s_q^2$, is strictly the same as that used in my calculations.[4] If both s orbitals in the $[p,(s,s)^3S]$ partial wave are orthogonalized to the $1s_q$ orbital, then this partial wave is orthogonal to all configurations of the form $1s_qnsn'p$. Note that these configurations can represent the open channels associated with all singly excited S states of the target. Hence, this orthogonality is too strong; it is rather proper for triply excited resonances. In fact, the "effective" principal quantum numbers of s electrons in the $[p,(s,s)^3S]$ partial wave are equal to 2 or greater. That is probably why the contribution of this partial wave to the resonance energy is, in Chung's calculation,[2] almost twice less than in mine. Thus, this choice of *auxiliary* holes is not efficient. Perhaps it would be better to orthogonalize two s orbitals in $[(s,s)^3S,p]$ to the $2s_q$ orbital. The other way, probably the best among the *auxiliary* hole projections, is to orthogonalize one of s orbitals to both $1s_q$ and $2s_{q'}$. In this way the $[(s,s)^3S,p]$ partial wave would be orthogonal to $1s_q2s_{q'}np$ configurations, which represent the open channel connected with the target $2\ ^3S$ state as well as the closed channel connected with the $2\ ^1S$ state. In my calculation[4] this representation is similar but, because the symmetry of the target is taken into account, only the open channel is projected out. Moreover, in the generalized saddle-point method, the "proper node structure" of orbitals is *implicitly* incorporated due to the symmetry of the target $(1s2s)^3S$ function. This may be shown as follows. Suppose that, instead of an arbitrary $2s$ orbital, one uses the orbital

$$|2s'\rangle \equiv |2s\rangle - |1s\rangle\langle 1s|2s\rangle\ ,$$

having the proper node structure. Then the spatial part of the $(1s2s')^3S$ function is

$$\det\{1s2s'\} = \det\{1s2s\} - \langle 1s|2s\rangle \det\{1s1s\}$$
$$= \det\{1s2s\}\ ,$$

which is the same as that with $2s$ used. Thus, in my calculation, the $2s$ orbital has, effectively, the "proper node structure." On the other hand, this structure should be *explicitly* included in hole-projection calculations. However, as it has been found by Jaskólska and Woźnicki,[8] the node structure of the $2s_q$ orbital very slightly influences the resonance energy.

The orbital hole-projection technique and the generalized saddle-point method have a common base. Both of them can be derived from the mini-max principle. They consist in orthogonalization of the trial function to an approximate open-channel space which is optimized to maximize the resonance energy. However, there are some differences between them.

(i) In the *generalized method* the Feshbach-type projectors are used, which is the best method of orthogonalization to the open-channel space. (Note that the well-defined forms of these projectors for three-electron or larger systems have been known[9] since 1985.) In Chung's method, the orthogonality to the open-channel space is obtained implicitly by a specific orthogonalization of orbitals.

(ii) There is no formal limitation for the target-state wave functions in the *generalized method.* In particular, configuration-interaction wave functions can be used. On the other hand, the target-state description in the hole-projection technique is limited by the way the vacancies are built in. Usually this description cannot be better than the one-configurational one.

(iii) $He^-\ 1s2s2p\ ^2P^\circ$-like cases can be handled by the *generalized* saddle-point method in a natural way, without any additional constraints required.

(iv) Energies of triply excited states, as those reported by Chung[2] can be also easily calculated with the *generalized* saddle-point method. In a recent article[10] I have introduced Feshbach-type projections for multiply excited resonances. They can be used within the generalized saddle-point method. For lithiumlike triply excited states, the generalized method is strictly equivalent to the hole-projection technique (as in the case of doubly excited states in two-electron systems). However, for systems containing more than three electrons, the *generalized* saddle-point method has the same formal advantages as in the case of doubly excited resonances, (i)–(iii). For example, if in the case of the berylliumlike $1s2s2p2p\ ^3P$ resonance, the $1s_q$ hole is built into the trial function then the trial function is made orthogonal to $1s_q^2nln'l'$ functions which represent the open-channel space. The two-electron core characteristic of the open-channel wave functions is described by only one configuration, $1s_q^2$. In the *generalized method* this core can be described by a configuration-interaction wave function.

Finally, I would like to emphasize that the main aim of my previous work, Ref. 4, was to properly interpret the hole-projection method. The generalized saddle-point method is a natural generalization of the original Chungs method which enables us to determine the relationship of the latter method to the deep-rooted Feshbach projection method. Although the generalized method is more expensive than the hole-projection technique, it is also suitable for practical application, especially for those cases where the "inner-shell-vacancy picture" is unclear.

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