Comments

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Comment on "Generalized saddle-point method for Feshbach resonances"

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In the recent article by M. Bylicki [Phys. Rev. A **39**, 3316 (1989)], many remarks were made concerning the saddle-point technique developed by this author. These remarks appear to have been based on a misunderstanding of both the spirit as well as the actual application of this method. In this Comment, I shall try to clarify some of these misunderstandings, and one hopes, put the problem in its proper perspective.

The saddle-point technique was developed by Chung in 1979.[1] In the past ten years, the method has been applied to numerous two- and three-electron systems.[2] In the course of application, some well-accepted interpretations of experiments were challenged.[3,4] Many heretofore unidentified Auger lines seen in existing experiments were identified.[5,6] While I have never claimed the method to be exact, the precision of our results had led to the recalibration of several high-resolution Auger spectra in which experimental absolute calibration is difficult.[7] Perhaps one of the most remarkable successes is the unambiguous identifications of some lithiumlike triply excited states arising from ion-atom or ion-molecule collisions.[8] Here the selection rules break down and many assorted triply excited states are produced in the collision experiment. Many of the resonances have several decay channels, thus further complicating the Auger spectra. These identifications have not been challenged by other methods. This saddle-point method is further incorporated with the complex-rotation method[9] to calculate the Auger width[10] or the spin-induced width[11] of atomic ions. Many of these predictions were verified by precise experiments.[12]

However, very recently, Bylicki claimed that "there are many instances in which it does not work."[13] This claim is based on the example of He^- $1s2s2P\ ^2P$ for which he added 15 $[(s,s)^3,p]^2P$ terms to the wave function. He was able to decrease the energy of this state by 0.000 099 a.u. (2.69 meV) and therefore these terms are not negligible as I have suggested.[3] On the other hand, including this partial wave in the wave function will lead to variation breakdown in his saddle-point calculation. This is due probably to misunderstanding of the application of this method.

He^- $1s2s2p\ ^2P$ is a broad resonance with a width of about 500 meV.[14] The methods Bylicki and I have used are approximations in which the interaction with the open-channel segment are neglected. As I explained in Ref. 3 (Sec. V), the shift of the resonance position for this state will be large. I will not be surprised if this shift turns out to be about 200 meV and therefore the result will agree with the scattering calculation[15] or complex-rotation calculation[16] when this shift is included. One can always debate the "vital importance"[13] of 2.69 meV when 200 meV is already neglected. But, there is a more basic reason why I did not include this $[(s,s)^3,p]$ partial wave at the time. This is related to the historical interpretation of He^- $1s2s2p\ ^2P$.

Before Ref. 3 was published, it was commonly believed by experimentalists and theoreticians alike that this $He^-\ ^2P$ state was a shape resonance associated with the $(1s2s)^3S$ open channel. I was using a new, but not yet popularly accepted, method to challenge a well-accepted concept. I claimed that this resonance was formed by the strong coupling of $[(1s2s)^1,2p]$ and $[(1s2p)^1,3d]$ rather than the $(1s2s)^3S$ channel. Therefore, I wanted to use a wave function that was orthogonal to the $(1s2s)^3S$ channel *by symmetry* so as to show this resonance arises in the complete absence of this open channel. Also, I needed a wave function that Temkin's quasi-projection-operator method[17] in its simplest form can use to obtain the same conclusion. The latter reason was a central point of my previous publication. Reference 3 did not concern the accuracy of a few meV, rather, the nature of this resonance.

The saddle-point method does not encounter a problem when this $[(s,s)^3S,p]$ is used. The effectiveness of the method lies in the ever-important fact that one builds the

TABLE I. Energy convergence of $1s2s2p\ ^2P^\circ$ He^- (in a.u.). ΔE is the binding energy contributed by adding the partial wave; for the detailed form of the wave function, see Ref. 3.

Partial wave	No. of terms	Nonlinear parameters			$-\Delta E$
$[(s,s)^1S,p]$	38	2.0	0.54	0.345	2.141 133
$[(s,p)^1P,d]$	4	2.0	0.515	0.42	0.006 308
$[(s,s)^3S,p]$	17	1.1	0.39	0.905	0.000 056
$[(p,p)^1S,p]$	5	2.0	1.6	0.24	0.000 859
$[(s,d)^1D,p]$	3	2.0	0.44	0.77	0.000 608
$[(d,d)^1S,p]$	2	2.9	3.0	0.25	0.000 066
$[(p,d)^1P,d]$	1	1.6	1.84	0.37	0.000 034
$[(s,d)^1D,f]$	1	2.0	0.69	0.87	0.000 033
Total					2.149 097

correct physics into the wave function. Since the system lies in the inelastic channel, one must build the proper vacancy such that the open channel is removed. This open channel is of the form of $[(1s2s)^3S,kp]$. Therefore, one must not allow the two s electrons in this $[(s,s)^3S,p]$ partial wave to form a $1s$ and another $2s$ orbital simultaneously. There are a number of ways to accomplish this purpose when this partial way is used. Notice that in all my discussions of the hole projection operators, the antisymmetrization is taken *after* the projection is done. Therefore, if one wishes to define a single projection operator for the total wave function, one only has to define the projection operator as

$$(1-|\varphi_{1s}(2)\rangle\langle\varphi_{1s}(2)|)(1-|\varphi_{1s}(3)\rangle\langle\varphi_{1s}(3)|)$$

and write the partial wave as $[p,(s,s)^3S]$. When we leave all the other parts of the wave function the same, the variation calculation can be carried out, there will be no breakdown. To illustrate, I carried out a calculation with this approach. A 17-term $[p,(s,s)^3]$ partial wave is used with no term selection. This result is given in Table I. We found a contribution of 0.000 056 a.u. which is a slightly smaller contribution than that of Ref. 13. It is difficult to judge which result is more reliable because of the severe approximate nature of the target states used in Ref. 13. The $1s2s\ ^3S$ basis function does not even have the proper node structure, not to mention radial or angular correlation. If Ref. 13 can use a much more flexible target basis, it is likely that his result may agree better with this work. In any case, I did not obtain a "spurious" result as suggested by Bylicki.[13] Regardless of whether one likes this procedure, one should not lose sight of the fact that we are discussing a partial wave which contributes 2 meV when more than 200 meV is neglected. How one deals with this partial wave is not important when the open channels are included in obtaining the correct resonance position. I fail to see the "vital importance" mentioned in Ref. 13.

Bylicki stated that, "The proof of Ching's theorem for a many-particle system is unsatisfactory." It should be emphasized that I do not have a "theorem" for a many-particle system.

I tried very hard to explain the mathematical and physical foundations of the saddle-point technique in the conclusion of Ref. 1 and more explicitly on p. 76 of Ref. 2. I emphasized that it is based on the variation principle of quantum mechanics and the validity of the "inner-shell-vacancy picture." Therefore, I did not "derive" this method. I generalized the result of the one-electron theorem to the many-particle system simply to indicate that one should search for a certain maximum in the variation procedure. The projection operator for each application must depend on the physics of that problem. The accuracy of this method depends on whether the "inter-shell-vacancy picture" is an accurate description of the physical reality. In fact, this shift of 200 meV of $He^-\ ^2P$ may very well be an indication that this "inner-shell-vacancy picture" is not an accurate description of the system. (Judging from Bylicki's result,[13] the "generalized saddle-point method" fares no better.) However, in the case that the resonance does not lie very close to an open channel, the accuracy of results never ceases to amaze me. I have recently extended the calculations to four-electron systems. The results obtained thus far indicate to me that many interesting identifications will be made in the four-electron Auger spectra.

Bylicki stated correctly that the hole projection is a method of building vacancy not a method of orthogonalization. As is well known, because of the Pauli antisymmetry principle, an exact Feshbach projection operator P or Q for three or more electrons does not exist in closed form. For this reason, I never tried to define a P space for orthogonalization. Rather, according to the physics of the system, I consider that the wave function should consist of two parts. The closed-channel part consists of appropriate holes. The open-channel part consists of no holes similar to that of the closed channel. Hence, if the holes are built in correctly there should be no continua in the closed-channel wave function. In this sense, orthogonality is achieved automatically. We have actually checked a few cases in which resonance is not very close to an open channel, orthogonality is achieved to an amazing degree.[10]

This seeming "weakness" of the saddle-point method is precisely where the strength of the method lies. What it means is that I do not need to worry about the target-state wave functions in the P space which are different for each and every problem. To calculate any resonance is just the same as bound-state configuration-interaction (CI) calculation. A uniformly applicable computer code

can be constructed. With very limited resources we have generated numerous results in a few years, the primary reason being the simplicity of the method. An interesting feature we found is that the structure of the vacancy orbital is very simple. At one time I tried to make it more complex, hence, more flexible, but the result does not change appreciably.

Bylicki[13] has proposed a method to project out the P space. If projecting out the P space is of such importance then P must be defined accurately. In Bylicki's calculation, the two-electron targets are defined by a one-term function (with symmetrization). It is not clear why the radial and angular correlations are not included, or why it is not important. It is also not clear whether it is feasible to apply this method with a correlated target-state wave function (e.g., with 20-term three angular-partial waves).

Bylicki stated that, "Difficulties appearing in the hole-projection technique do not occur in the generalized saddle-point method." This gives the impression that the "generalized" method must have a wider applicability than the restrictive method developed by myself. The restrictive method can generate a high-precision result for important resonances such as lithium-like $2s2s2p\ ^2P$ (Ref. 2) or beryllium-like $1s2s2s2p\ ^3P$ or $1s2s2p2p\ ^3P$ (Ref. 18) where infinite open channels exist. How to project out the infinite numbers of open-channel target states from the total wave function would be an interesting question. If this cannot be done easily, perhaps the word "generalized" is somewhat misleading.

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