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Comment on "Weyl's theory and the complex-rotation method applied to phenomena associated with a continuous spectrum"

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Recent computations of complex-energy resonance poles by Rittby, Elander, and Brändas for a $V(x)=(\frac{1}{2}x^2-J)e^{-\lambda x^2}+J$ model potential are compared with results found by a recently developed alternative technique using Milne's method. Differences in the resulting behavior of the pole string are discussed.

In a recent interesting article[1] a new method has been presented for the computation of complex-energy (Siegert) poles of the S matrix. The method combines Weyl's theory and the complex-rotation method. The authors illustrate the capability of their technique by calculated resonance positions in the complex-energy plane for the potential

$$V(x)=(\tfrac{1}{2}x^2-J)e^{-\lambda x^2}+J,\quad J=0.8,\ \lambda=0.1, \tag{1}$$

previously studied by Moiseyev *et al.*[2] These results seem to be the first published computation of a complex-energy pole string of about 40 complex resonances obtained numerically for a fairly general potential.

Different numerical methods with comparable efficiency have been developed independently by Atabek *et al.*,[3,4] who use the finite difference boundary value method, and the present authors,[5–7] who make use of Milne's differential equation. Both methods are also based on the complex-rotation method.

Almost analytical results have been obtained for a small number of simple cases, including square-well,[8,9] Coulomb,[10,11] surface delta,[12] Morse,[13] and inverse Kratzer—or Fues—[$V(r)=a/r-b/r^2$; $a,b>0$] (Ref. 14) potentials.

Rittby *et al.*,[1] furthermore, define a "complex threshold," based on the quite unexpected finding, that the real part E_R of the resonance energy $E(n)=E_R(n)+iE_I(n)$ is bounded from above for the potential (1), i.e., there exists a "complex threshold" E_{thresh}, such that $E_R(n)\leq E_{\text{thresh}}$ for all n. This suggests a natural partitioning of the poles in two classes: those before and behind the threshold (compare Fig. 1 of Rittby *et al.*[1]), eventually related to resonances structures and background in the energy dependence of the cross sections as speculated by Rittby *et al.*[1]

It is the purpose of this Comment to point out that the computational results by Rittby *et al.*[1] above the complex threshold show a behavior which is inconsistent with recent observations of the present authors for the potential

$$V(r)=V_0r^2e^{-r}, \tag{2}$$

where the pole string also shows a complex threshold behavior, but, contrary to the findings of Rittby *et al.*,[1] the real part $E_R(n)$ is monotonically decreasing for resonances above the threshold, whereas the resonances computed by Rittby *et al.*[1] for potential (1) show an oscillatory behavior of the real part.

We therefore computed the resonances for potential (1) by our complex-rotated Milne method. The resulting pole string is plotted in Fig. 1 and the resonances for odd values of n are given in Table I. In Fig. 1 the pole string shows exactly the same behavior as observed for potential (2) in disagreement with the results by Rittby *et al.*,[1] which may be due to numerical instabilities in their computations or a consequence of a too limited range of variation of the complex-rotation angle $\eta\,(0<\eta<\pi/4)$. In our calculations we used rotation angles up to $\eta=50°$.

In order to check the validity of the resonance positions computed by our complex-rotated Milne

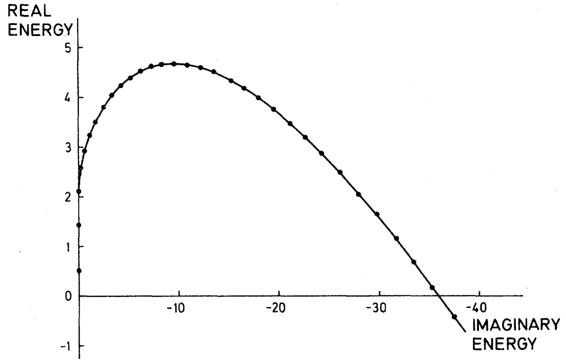

FIG. 1. Complex-energy resonance poles for the potential (1) ($\hbar=m=1$) computed by means of the complex-rotated Milne method.

TABLE I. Complex-energy resonance poles $E(n)=E_R(n)+iE_I(n)$ for the potential (1) ($\hbar=m=1$) for odd values of n. Exact numerical results computed by means of the complex-rotated Milne method are compared with a semiclassical (WKB) approximation.

	Exact		WKB	
n	E_R	E_I	E_R	E_I
1	1.4210	-0.5828×10^{-4}	1.4413	-0.5408×10^{-4}
3	2.5846	−0.1738	2.6067	−0.1715
5	3.2555	−1.1115	3.2760	−1.1067
7	3.8243	−2.4874	3.8432	−2.4816
9	4.2500	−4.1832	4.2674	−4.1770
11	4.5288	−6.1547	4.5452	−6.1487
13	4.6619	−8.3756	4.6769	−8.3693
15	4.6441	−10.8263	4.6640	−10.8195
17	4.5199	−13.4658	4.5081	−13.4846
19	4.1968	−16.3581	4.2109	−16.3529
21	3.7601	−19.4198	3.7727	−19.4139
23	3.1850	−22.6670	3.1975	−22.6614
25	2.4730	−26.0929	2.4853	−26.0875
27	1.6252	−29.6913	1.6374	−29.6861
29	0.6429	−33.4570	0.6551	−33.4519
31	−0.4729	−37.3852	−0.4607	−37.3803

method, we have also carried out approximate WKB calculations of the complex-energy resonances. This semiclassical approximation[6,7] is not based on the complex-rotation method and, as expected, the results are in good agreement with the values given by the complex-rotated Milne method. Therefore we suspect that the higher resonances computed by Rittby *et al.*[1] are incorrect.

Finally, we point out that the effect of narrow and isolated poles on the scattering phase shift and the partial cross section is well understood, but, particularly in view of the currently increasing interest in complex-energy resonance states, there is a basic need in the understanding of the typical behavior of the full pole string (the "polology") for interatomic or intermolecular potentials with nonisolated overlapping resonances, as well as the implications on observable (real energy) effects. Some work along these lines is in progress and will be published elsewhere.[13]

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[1] M. Rittby, N. Elander, and E. Brändas, Phys. Rev. A 24, 1636 (1981).

[2] N. Moiseyev, P. R. Certain, and F. Weinhold, Mol. Phys. 36, 1613 (1978).

[3] O. Atabek, R. Lefebvre, and A. Requena, Mol. Phys. 40, 1107 (1980).

[4] O. Atabek and R. Lefebvre, Chem. Phys. Lett. 84, 233 (1982).

[5] H. J. Korsch and H. Laurent, J. Phys. B 14, 4213 (1982).

[6] H. J. Korsch, H. Laurent, and R. Möhlenkamp, J. Phys. B 15, 1 (1982).

[7] H. J. Korsch, H. Laurent, and R. Möhlenkamp, Mol. Phys. 43, 1441 (1981).

[8] H. M. Nussenzveig, Nucl. Phys. 11, 499 (1959).

[9] S. Joffily, Nucl. Phys. A215, 301 (1973).

[10] C. Moller, K. Dan. Vidensk. Selsk. Mat. Fys. Medd. 22, No. 19 (1946).

[11] E. M. Ferreira and A. F. F. Teixeira, J. Math. Phys. (N.Y.) 7, 1207 (1966).

[12] W. J. Romo, Can. J. Phys. 52, 1603 (1974).

[13] H. J. Korsch and R. Möhlenkamp (unpublished).

[14] G. D. Doolen, Int. J. Quantum Chem. 14, 523 (1978).