Response to ''Comment on 'On the direct complex scaling of matrix elements expressed in a discrete variable representation: Application to molecular resonances' '' [J. Chem. Phys. 109, 1201 (1998)]

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As emphasized in our original paper,[1] the main purpose of the proposed method is to numerically continue the matrix elements of a multidimensional Hamiltonian operator expressed in a contracted basis set of the type

$$\{|\Phi_m(R_p)\rangle|R_p\rangle, m=1,M_p; p=1,P\}.$$

In the above notation, the $\{|R_p\rangle\}$ stand for some discrete variable representation (DVR), and the $\{|\Phi_m(R_p)\rangle\}$ represent the adiabatic solutions computed at fixed value $R=R_p$. As this procedure requires the numerical continuation of the potential matrix elements initially expressed in a grid representation, we first presented results for the one-dimensional (1D) test case considered by Bludsky *et al.* However, contrary to what is claimed in their comment, we show below that for this test case

(i) our method actually leads to a much better precision than the one reported in their Table I;

(ii) it does not fail when larger basis sets are used;

(iii) the correction proposed by these authors [Eq. (10)] cannot be used as their basic assumption [Eq. (9)] does not hold.

We compare in Table I below the results obtained using our original method, those of Bludsky *et al.*, as well as the values computed by means of an analytical continuation. In all cases, the same basis set of 29 DVR points covering the range $R\in[0,15]$ has been used. However, Bludsky *et al.* mention using 200 integration points in their calculation, as compared to 58 in ours. Due to the numerical continuation, the complex trajectories display a more scattered behavior than when using analytical continuation, as shown in Fig. 1. The resonance position is then ascribed to the rapid departure from a stationary behavior. From this figure, the resonance characteristics for E_1^-, as obtained from numerical continuation, display 8 and 4 digits of accuracy for the position and width, respectively; for E_3^-, the accuracy is of 7 and 6 digits, respectively.

Figure 2 displays the complex trajectories, as obtained

TABLE I. Results for the first two odd resonances of the one-dimensional Hamiltonian model $H=-\frac{1}{2}d^2/dR^2+(R^2-J)e^{-\lambda R^2}+J$, where $J=0.8$ and $\lambda=0.1$. A basis set of 29 DVR points covering the range $R\in[0,15]$ has been used.

	Numerical continuation		
	Our method[a]	Bludsky *et al.*[b]	Analytical continuation
$\mathrm{Re}[E_1^-]$	1.420 971 01	1.421	1.420 970 99
$\mathrm{Im}[E_1^-]$	$-5.8268(-5)$	$-5.828(-5)$	$-5.8272(-5)$
$\mathrm{Re}[E_3^-]$	2.584 584	2.5846	2.584 583
$\mathrm{Im}[E_3^-]$	$-1.737\,51(-1)$	$-1.7375(-1)$	$-1.737\,508(-1)$

[a]Using 58 integration points.
[b]Using 200 integration points.

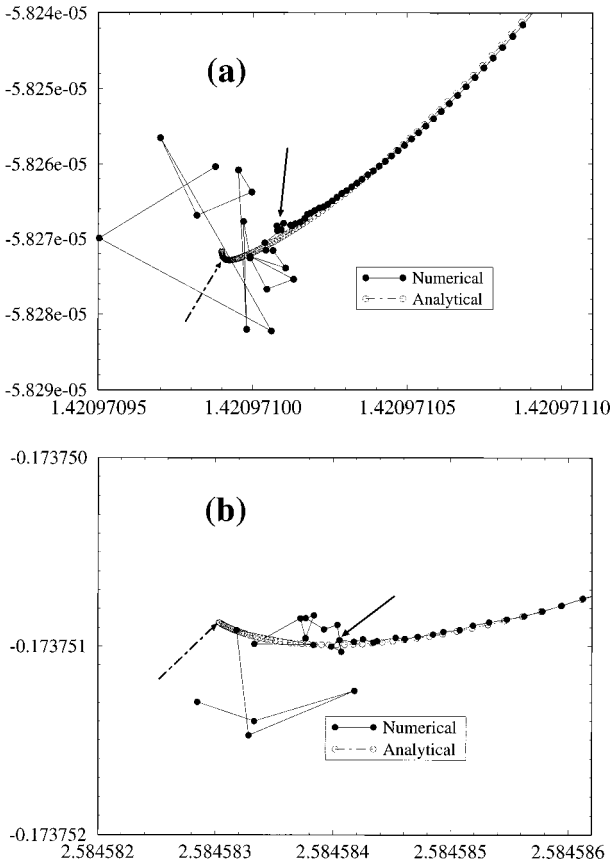

FIG. 1. Complex trajectories associated to the two resonances reported in Table I, as obtained by numerical (●—●) or analytical (o_._o) continuation : (a) E_1^- ; (b) E_3^- . The arrows indicate the resonance location.

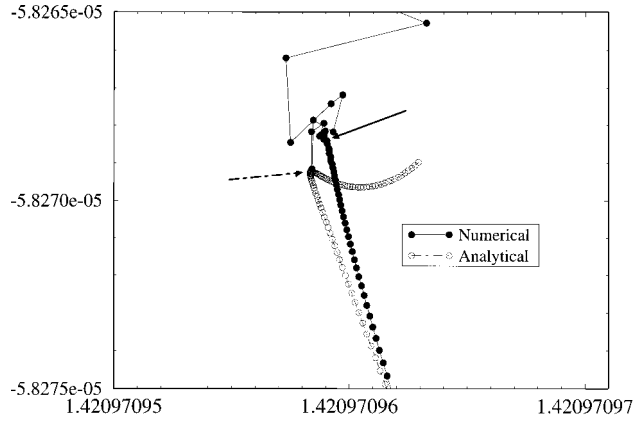

FIG. 2. Same as Fig. 1(a) for a basis set of 39 grid points covering the range $R \in [0,20]$.

by using a larger basis set of 39 grid points covering the range $R \in [0,20]$, and computed by numerical and analytical continuations. Only the first E_1^- resonance is shown in this figure. The results displayed in Table II demonstrate that the resonance is now computed to 9 digits of accuracy for the position, the width being known with 5 significant digits.

In their comment, Bludsky *et al.* propose to take into account the integration along the contour Γ_∞ running from

TABLE II. Results for the E_1^- resonance as computed with a basis set of 39 DVR points covering the range $R \in [0,20]$.

	Numerical continuation[a]	Analytical continuation
$\mathrm{Re}[E_1^-]$	1.420 970 959	1.420 970 958
$\mathrm{Im}[E_1^-]$	$-5.8268(-5)$	$-5.8269(-5)$

[a]Using 78 integration points.

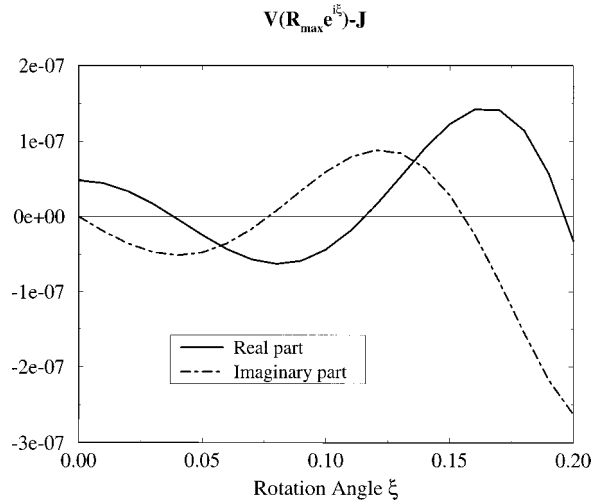

FIG. 3. Variation of the quantity $V(R_{\max}e^{i\xi})-J$ along the contour Γ_∞ (see text), as a function of the rotation angle ξ.

$R_{\max}$ to $R_{\max}e^{i\theta}$ as stated in their Eq. (8). To this end, they make the assumption that $V(R_{\max}e^{i\xi})$ can be approximated by some constant V_0 along this contour Γ_∞. It should, however, be noted that they never mention which value V_0 was actually used in the subsequent calculations. To test this assumption, we report in Fig. 3 the values taken by the quantity $V(R_{\max}e^{i\xi})-J$ along this contour Γ_∞, as a function of the rotation angle ξ. The constant $J=0.8$ has been subtracted in order to show the actual variation. Looking at this figure, it seems difficult to define a meaningful V_0 approximation, other than the trivial one $V_0=0$. This simply corresponds to ignoring the contribution along the contour Γ_∞, as was implicitly done in our original method.

[1] K. Museth and C. Leforestier, J. Chem. Phys. **107**, 7008 (1996).