Partial widths obtained by the complex resonance-scattering theory

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A complex resonance-scattering theory is developed to obtain partial widths and branching ratios for full scattering experiments. A new formula for the partial widths which is useful in atomic, molecular, nuclear, and particle physics is obtained. The formalism provides a simple relationship among the previously proposed different methods for calculating partial widths. Illustrative numerical examples are given, showing the stability (lack of oscillations) of the partial widths obtained by this formula.

I. INTRODUCTION

While resonances are the "most striking phenomenon in the whole range of scattering experiments,"[1] probably the resonance partial widths—the calculation and measurement of which are used to compare theory with experiment—are the most significant output of the resonance phenomenon. Partial widths represent the probability per unit time of getting a specific reaction product in a well-defined quantum state in a full scattering or half-collision experiment.

Different square-integrable wave-function methods for obtaining the partial widths of the resonant decay into individual channels were described in the literature.[2,3] Two different procedures based on the complex coordinate method (CCM) were proposed by Noro and Taylor[4] and by Bačić and Simons.[5] A third method, similar to that of Bačić and Simons, based on the analysis of the tail of the complex scaled square-integrable resonance wave function, was proposed by Peskin, Moiseyev, and Lefebvre.[6] This very simple approach does not require any integration over the channel functions. Knowledge of the resonance functions at some point in the asymptotic region is sufficient to yield the rates of decay.[6]

The purpose of this paper is to represent a coherent complex resonance-scattering theory linking the different methods for calculating partial widths. The theory provides the conditions for the applicability of these methods and leads to a derivation of a new formula for partial widths and branching ratios.

II. PARTIAL WIDTHS FOR A FULL SCATTERING EXPERIMENT

The Hamiltonian we shall study is

$$\hat{H}(\mathbf{x},r)=\hat{T}(r)+\hat{h}(\mathbf{x})+\hat{V}(\mathbf{x},r)\ , \tag{1}$$

where

$$\hat{T}(r)=-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial r^2}\ ,$$

$\{\mathbf{x}\}$ are the internal (or target) coordinates and $\hat{V}(\mathbf{x},r)$ describes the interaction potential of the scattered particle and the target, or the potential interaction of a specific molecular mode with other internal degrees of freedom. The eigenfunctions of the Hamiltonian are given by

$$\psi(\mathbf{x},r)=\sum_{j'}\chi_{j'}(\mathbf{x})\phi_{j'}(r)\ , \tag{2}$$

where $\chi_j(x)$ are the eigenfunctions of $\hat{h}(\mathbf{x})$,

$$[\hat{h}(\mathbf{x})-\varepsilon_j^{[x]}]\chi_j(\mathbf{x})=0\ . \tag{3}$$

By substituting $\psi(\mathbf{x},r)$ in the time-independent Schrödinger equation one can get a set of coupled equations given by

$$\underline{H}\boldsymbol{\phi}=E\boldsymbol{\phi}\ , \tag{4}$$

where E denotes the total energy of the system and

$$\hat{H}_{ii}=\hat{T}_r+\hat{V}_{ii}(r)+\varepsilon_j^{[x]}\ ,$$
$$\hat{H}_{ij}=\hat{V}_{ij}(r),\quad \hat{V}_{ij}=\langle\chi_i|\hat{V}(\mathbf{x},r)|\chi_j\rangle\ .$$

If $E<\varepsilon_j^{[x]}$, then the channel j is a closed channel and if $E>\varepsilon_j^{[x]}$, then j is an open channel for dissociation. In a scattering process the initial-i and final-f states are eigenfunctions of $\hat{h}(\mathbf{x})+\hat{T}(r)$:

$$|i\ (j_0)\rangle=e^{ik_{j_0}r}\chi_{j_0}(\mathbf{x})\ ,$$
$$|f\ (j)\rangle=\phi_j^{(f)}(r)\chi_j(\mathbf{x})\ , \tag{5}$$
$$\phi_j^{(f)}(r)=\sqrt{\mu/\hbar k_j}\,e^{ik_j r}\ ,$$

where $\phi_j^{[f]}$ is normalized to a unit current density such that

$$\frac{1}{2\mu}\{\langle\chi_j|[\phi_j^{(f)}(r)]^*\hat{p}_r\phi_j^{(f)}(r)$$
$$-\phi_j^{(f)}(r)\hat{p}_r[\phi_j^{(f)}(r)]^*|\chi_j\rangle\}=1\ .$$

$\hat{p}_r$ is the linear momentum operator, and $\hbar k_j$ is the linear momentum of the particle scattered to the channel j such that

$$\frac{(\hbar k_j)^2}{2\mu}=E-\varepsilon_j^{[x]}\ . \tag{6}$$

The probability to get from $|i\rangle$ to $|f\rangle$ in unit time is

given by

$$\Gamma_{j\leftarrow j_0} \propto |\langle f(j)|\hat{V}(1+\hat{G}_E\hat{V})|i(j_0)\rangle|^2 , \tag{7}$$

where $\hat{V}(1+\hat{G}_E\hat{V})$ is the usual T operator.

By carrying out the integration in Eq. (7) along a contour in the complex coordinate plane, $r\rightarrow r\exp(i\theta)$,[7-10] the familiar Green's operator takes the form

$$G_E=\sum_i \oint \frac{|\psi_i^\theta\rangle\rangle\langle\langle\psi_i^\theta|}{E-E_i^\theta}dE_i^\theta \tag{8}$$

or

$$G_E\equiv[\hat{H}(\mathbf{x},re^{i\theta})-E]^{-1} ,$$

the potential $\hat{V}(\mathbf{x},r)$ takes the form $\hat{V}(\mathbf{x},re^{i\theta})$, and

$$|i^\theta(j_0)\rangle=\exp[ik_{j_0}r\exp(i\theta)]\chi_{j_0}(\mathbf{x}) ,$$

$$|f^\theta(j)\rangle=\phi_j^{(f)}(re^{i\theta})\chi_j(\mathbf{x}) .$$

The complex scaled eigenfunctions $|\psi_i^\theta\rangle\rangle$ are given by

$$\hat{H}(\mathbf{x},re^{i\theta})|\psi_i^\theta\rangle\rangle=E_i^\theta|\psi_i^\theta\rangle\rangle . \tag{9}$$

According to the complex coordinate method, at a resonance state, $E_i^\theta=E_r-i\Gamma/2=E_{\rm res}$ and is θ independent. $\psi_{\rm res}^\theta$ is a square integrable function, whereas $\psi_{\rm continuum}^\theta\rightarrow\psi_{\rm continuum}^{\theta=0}$ as $r\rightarrow\infty$ and

$$E_{\rm continuum}^\theta=|E_{\rm continuum}^{\theta=0}-\varepsilon_j^{[x]}|e^{-2i\theta} ,$$

$\langle\langle\ |\ \rangle\rangle$ standing for the C product.[11,12] If a real basis set is used then $\langle\langle f|g\rangle\rangle=\langle f^*|g\rangle=\int fg\,d\tau$. If a complex basis set is used then the matrix element of given operator $\hat{O}$ is given by $\langle\langle\psi_i^{\theta L}|\hat{O}|\psi_j^{\theta R}\rangle\rangle=\int\psi_i^{\theta L}O\psi_j^{\theta R}dr$, where $\psi_i^{\theta L}$ and $\psi_i^{\theta R}$ are the corresponding left and right eigenvectors of $\hat{H}(\mathbf{x},re^{i\theta})$. Let us consider the specific case of a resonance scattering, where (i) the scattering experiment is such that the total energy E is equal to the resonance position, $E=E_r$, and (ii) the distances of the point $(E_r,0)$ in the complex energy plane from the straight lines $|E-\varepsilon_j^{[x]}|e^{-2i\theta}$ are larger than $\Gamma/2$ [i.e., $(E_r-\varepsilon_j^{[x]})\sin(2\theta)\gg\Gamma/2$]. In such a case there is only one dominant term in the series expansion of the G operator given in Eq. (8) such that

$$\Gamma_{j\leftarrow j_0}\propto\left|\frac{-2i}{\Gamma}\langle\langle f^\theta(j)|\hat{V}(\mathbf{x},re^{i\theta})|\psi_{\rm res}^\theta\rangle\rangle\right.$$
$$\times\langle\langle\psi_{\rm res}^\theta|\hat{V}(\hat{x},re^{i\theta})i^\theta(j_0)\rangle\rangle$$
$$\left.+\langle\langle f^\theta(j)|\hat{V}(\mathbf{x},re^{i\theta})|i^\theta(j_0)\rangle\rangle\right|^2 . \tag{10a}$$

For narrow enough resonances, $\Gamma\ll E_r-\varepsilon_j^{[x]}$, it may happen that the contribution of the direct scattering event to the cross section is small relative to the contribution of the multiple-scattering events (i.e., $\hat{V}\hat{G}_E\hat{V}$ terms) (we shall return to the validity of this assumption later) and $\Gamma_{j\leftarrow j_0}$ is given by

$$\Gamma_{j\leftarrow j_0}\propto\left[\frac{2}{\Gamma}\right]^2|\langle\langle f^\theta(j)|\hat{V}(\mathbf{x},re^{i\theta})|\psi_{\rm res}^\theta\rangle\rangle$$
$$\times\langle\langle\psi_{\rm res}^\theta|\hat{V}(\mathbf{x},re^{i\theta})|i^\theta(j_0)\rangle\rangle|^2 . \tag{10b}$$

From the same initial state several different final states can be obtained. That is,

$$|i(j_0)\rangle\rightarrow\begin{cases}|f(j)\rangle\\|f(j')\rangle\\|f(j'')\rangle .\end{cases} \tag{11}$$

From Eq. (10b) and Eq. (11) one can get

$$\frac{\Gamma_j}{\Gamma_{j'}}=\left|\frac{\langle\langle f^\theta(j)|\hat{V}(\mathbf{x},re^{i\theta})|\psi_{\rm res}^\theta\rangle\rangle}{\langle\langle f^\theta(j')|\hat{V}(\mathbf{x},re^{i\theta})|\psi_{\rm res}^\theta\rangle\rangle}\right|^2 . \tag{12}$$

This is the expression proposed by Noro and Taylor[4] for the calculation of branching ratios. We omit here the label j_0 since under the two assumptions leading from Eq. (7) to Eq. (10) we get that the only intermediate state in the scattering process is the resonance state. This is a result of neglecting both the direct scattering and the background contributions to the T matrix. The physical interpretation of the resonance scattering becomes clear. While the total energy (i.e., the sum of the particle and target energies) is taken as the resonance position, the initial state is "forgotten" during the scattering process. This is probably true in a half-collision process when the system is initially prepared in a resonance state.

In Eq. (12) the *complex* energy is not conserved since $|f\rangle$ is associated with the real energy $E-E_r$ whereas $|\psi_{\rm res}^\theta\rangle$ is associated with the complex energy $E_r-i\Gamma/2$. *We postulate that in the complex scattering theory the complex energy is conserved and therefore we introduce the complex momentum for the final state determined by*

$$\frac{(\hbar k_j)^2}{2\mu}=E_r-\frac{i\Gamma}{2}-\varepsilon_j^{[x]} . \tag{13}$$

Note that the kinetic energy is not equal to $E_r-\varepsilon_j^{(x)}$ as stated before in Eq. (6).

Therefore

$$\hat{T}(r)\phi_j^{(f)}(r)=\left[E_r-\frac{i\Gamma}{2}-\varepsilon_j^{[x]}\right]\phi_j^{(f)}(r) . \tag{14}$$

Also note that in the radial case where $r\in[0,\infty]$, $\phi_j^{(f)L}(re^{i\theta}=0)=0$, and yet

$$\phi_j^{(f)L}(re^{i\theta})\rightarrow\sqrt{\mu/k\hbar}\,e^{-ik_jre^{i\theta}}\quad\text{as } r\rightarrow\infty . \tag{15}$$

Therefore, in the *radial* case,

$$\phi_j^{(f)L}(re^{i\theta})=-2i\sqrt{\mu/k_j\hbar}\sin(k_jre^{i\theta}) . \tag{16}$$

Equation (12) can be rewritten by making use of the following derivation:

$$\langle\langle f^{\theta}(j)|\hat{V}(\mathbf{x},re^{i\theta})|\psi^{\theta}_{\rm res}\rangle\rangle = \int_{\text{all space}} \chi_j^*(\mathbf{x})\phi_j^{(f)L}(re^{i\theta})[\hat{H}(\mathbf{x},re^{i\theta})-\hat{H}_0(\mathbf{x},re^{i\theta})]\psi^{\theta}_{\rm res}d\mathbf{x}\,dr$$
$$= \left[E_r-\frac{i\Gamma}{2}\right]\int_{\text{all space}}\chi_j^*(\mathbf{x})\phi_j^{(f)L}(re^{i\theta})\psi^{\theta}_{\rm res}d\mathbf{x}\,dr$$
$$-\int_{\text{all space}}\chi_j^*(\mathbf{x})\phi_j^{(f)L}(re^{i\theta})\left[\hat{h}(\mathbf{x})+e^{-2i\theta}\frac{\hat{P}_r^2}{2\mu}\right]\psi^{\theta}_{\rm res}d\mathbf{x}\,dr$$
$$= \left[E_r-\frac{i\Gamma}{2}-\varepsilon_j^{[x]}\right]\int_{\text{all space}}\chi_j^*(\mathbf{x})\phi_j^{(f)L}(re^{i\theta})\psi^{\theta}_{\rm res}d\mathbf{x}\,dr$$
$$-\frac{e^{-2i\theta}}{2\mu}\int_{\text{all space}}\chi_j^*(\mathbf{x})\phi_j^{(f)L}(re^{i\theta})\hat{P}_r^2\psi^{\theta}_{\rm res}d\mathbf{x}\,dr\ . \tag{17}$$

The resonance eigenfunction of the complex scaled Hamiltonian $\hat{H}(\mathbf{x},re^{i\theta})$ can be described by [see Eq. (2)]

$$\psi^{\theta}_{\rm res}=\sum_{\gamma}\chi_\gamma(\mathbf{x})\Phi^{\theta}_{\gamma}(r)\quad\text{where }\Phi^{\theta}_{\gamma}(r)\to 0\text{ as }r\to\infty\ . \tag{18}$$

By substituting Eq. (18) into Eq. (17), making use of Eq. (14), and carrying out integration by parts, one can get that

$$\langle\langle f^{\theta}(j)|\hat{V}(\mathbf{x},re^{i\theta})|\psi^{\theta}_{\rm res}\rangle\rangle=\frac{\hbar^2e^{-2i\theta}}{2\mu}\left[\phi_j^{(f)L}(re^{i\theta})\frac{d\Phi^{\theta}(r)}{dr}-\Phi^{\theta}_j(r)\frac{d\phi_j^{(f)L}(re^{i\theta})}{dr}\right]\Bigg|_a^{\infty}\ . \tag{19}$$

When $a=0$ in the radial case $r\in[0,\infty]$ and $a=-\infty$ for the one-dimensional case, $r\in[-\infty,\infty]$. Note that in the radial case $\Phi^{\theta}_j(0)=0$ and also $d\Phi^{\theta}_j(r)/dr|_{r=0}=0$, and only the upper limit, i.e., $r=\infty$, should be taken into consideration. Consequently, from Eqs. (12) and (18) one can get

$$\frac{\Gamma_j}{\Gamma_{j'}}=\left|\frac{\left[\phi_j^{(f)L}(re^{i\theta})\frac{d\Phi^{\theta}_j(r)}{dr}-\Phi^{\theta}_j(r)\frac{d\phi_j^{(f)L}(re^{i\theta})}{dr}\right]_a^{\infty}}{\left[\phi_j^{(f)L}(re^{i\theta})\frac{d\Phi^{\theta}_{j'}(r)}{dr}-\Phi^{\theta}_{j'}(r)\frac{d\phi_j^{(f)L}(re^{i\theta})}{dr}\right]_a^{\infty}}\right|^2\ . \tag{20}$$

This is a new formula for the branching ratio, where $\phi_j^{(f)R}(r)$ and $\phi_j^{(f)L}(r)$ are, respectively, the divergent outgoing and incoming plane waves with the complex momentum $[2\mu(E_r-i\Gamma/2-\varepsilon_j^{[x]})]^{1/2}$. Φ^{θ}_j is a square-integrable function from the variational solution of the Schrödinger equation associated with the resonance complex eigenvalue $E_r-i\Gamma/2$. The new partial width expression appears to be more compact (in dimensionality) than the older one [Eq. (12)] and thus avoids the need to integrate over the target coordinates $\mathbf{x}$. Note that[6]

$$\Phi^{\theta}_j(r)\to a_j\phi_j^{(f)}(re^{i\theta})\quad\text{as }r\to\infty \tag{21}$$

and therefore by substituting Eq. (21) into Eq. (20) one can get that

$$\frac{\Gamma_j}{\Gamma_{j'}}=\left|\frac{a_j}{a_{j'}}\right|^2\ . \tag{22}$$

Here $|a_j|^2$ provides the probability to decay into the open channel j. By taking into consideration Eq. (21) and the fact that $|a_j|^2$ is normalized to a unit current density, one can see that $|a_j|^2$ is actually the probability flux of $\Phi^{\theta}_j(r)$ at $r\to\infty$, namely, that the number of particles at the quantum state j detected at $r=\infty$ per unit time per unit area. a_j can be easily obtained by carrying out an asymptotic analysis of the resonance eigenfunction:

$$a_j=\lim_{r\to\infty}\left[\frac{\Phi^{\theta}_j(r)}{\phi_j^{(f)}(re^{i\theta})}\right]\ , \tag{23}$$

where

$$\phi_j^{(f)}(re^{i\theta})=\sqrt{\mu/\hbar k_j}\,e^{ik_j(re^{i\theta})}\ ,$$
$$\frac{(\hbar k_j)^2}{2\mu}=E_r-\frac{i\Gamma}{2}-\varepsilon_j^{[x]}\text{ where }\varepsilon_j^{[x]}\text{ is the threshold}\ .$$

Therefore the branching ratio is given by

$$\frac{\Gamma_j}{\Gamma_{j'}}=\lim_{r\to\infty}R(r)$$

where

$$R(r)=\left|\frac{(k_{j'})^{1/2}}{(k_j)^{1/2}}\frac{\Phi^{\theta}_j(r)}{\Phi^{\theta}_{j'}(r)}e^{i(k_{j'}-k_j)re^{i\theta}}\right|^2\ . \tag{24}$$

This formula has been proposed before by Peskin, Moiseyev, and Lefebvre and is closely related to the formula proposed by Bačić and Simons for the calculation of branching ratios.

In this section we show that there are simple relation-

ships among the different methods for calculating the partial widths and that the three different formulas for the branching ratio given in Eqs. (12), (20), and (24) are identical. Consequently, in the limit of infinite-basis-set variational calculations the same results for the partial widths should be obtained.

III. ILLUSTRATIVE NUMERICAL EXAMPLES

The three different formulas for calculating partial widths and branching ratios given by Eqs. (12), (20), and (24) are applied to two multichannel scattering problems studied before and used as test models for new theories.[4-6,13,14] In this section we are not aiming at presenting new results, rather at showing that indeed—as predicted by the complex resonance-scattering theory presented in Sec II—the same partial widths are obtained by using any of the three formulas mentioned above. The first model is a two-channel Hamiltonian studied by Noro and Taylor,[4] and by Bačić and Simons. The potential matrix elements are given by

$$V_{ij}(r)=\lambda_{ij}r^2\exp(-r)+E_{tj}\delta_{ij} \quad \text{for } r\in[0,\infty]$$

where

$$\lambda_{11}=1,\quad \lambda_{12}=\lambda_{21}=-7.5\quad \lambda_{22}=7.5\ .$$

The threshold energies are $E_{t1}=0$ and $E_{t2}=0.1$ Channel 2 of the potential, $V_{22}(r)$ supports a shape resonance, but because of the coupling to channel 1, the resonance has a dominant Feshbach-type character.

The second studied three-channel model Hamiltonian is of Yu and co-workers[15] for an HD molecule on an Ag(111) flat surface in the rigid rotor approximation:

$$H=-\frac{\hbar^2}{2M}\frac{d^2}{d\hbar^2}+B_{\rm rot}\hat{j}^2(\nu)+V(z,\gamma)\ .$$

Here γ is the orientation of the diatom, $\hat{j}$ is the rotational angular momentum, and $z\in[-\infty,\infty]$ is the distance of the HD center of mass from the Ag(111) surface. The HD/Ag(111) Feshbach-type predesorption resonances positions and widths were obtained as described in Refs. 13 and 14 by the complex coordinate method. In the two studied cases, N particle-in-a-box basis functions (L is the box length) were used to describe the dissociation along the reaction coordinate (r in the Noro-Taylor model and z, $(z\in[z_{\rm min},z_{\rm max}])$ in the HD/Ag(111) model Hamiltonian). N was taken as 80 and $L=16$ in the NT model and $N=75$, $L=z_{\rm max}-z_{\rm min}=19$ with $z_{\rm min}=-3$ in the HD/Ag model.

The two model Hamiltonians were complex scaled by

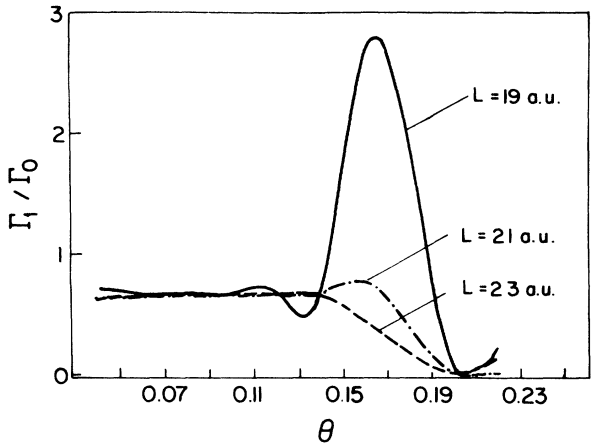

FIG. 1. Branching ratio $\Gamma_{J=1}/\Gamma_{J=0}$ of the $(V=4, J=2)$ HD/Ag(111) predesorption resonance obtained from Eq. (12) as a function of the rotational angle θ [the complex scaling factor is $\exp(i\theta)$] for different particle-in-a-box basis functions. L stands for the box size functions, and the label (V,J) is explained in the caption of Table I.

TABLE I. The resonance positions E_r, widths Γ, branching ratios Γ_1/Γ_0, and partial widths Γ_0 and Γ_1 for the Noro-Taylor two-channel model Hamiltonian, and for the scattering of HD from an Ag(111) surface are presented. The branching ratios and partial widths were obtained from Eqs. (12), (20), and (24). The label (V,J) stands for the bound state of the freely rotating HD molecule which becomes a resonance state (i.e., finite lifetime) as the coupling between the rotational motion of HD and the vibrational motion of the HD/Ag(111) complex is taken into consideration.

Model	Resonance	Formula	Γ_1/Γ_0	$\Gamma_0\times10^5$	$\Gamma_1\times10^5$	$(\Gamma_1+\Gamma_0)\times10^5$
Noro	$E_r=4.7682$	Eq. (12)	26.8	5.1	136.8	142
and		Eq. (20)	26.9	5.1	137.0	142
Taylor	$\Gamma=144\times10^{-5}$	Eq. (24)	27	5	145	150
	$(V=2, J=2)$	Eq. (12)	0.67	1.54	1.03	2.57
HD/Ag	$E_r=56.8\times10^{-5}$	Eq. (20)	0.67	1.53	1.03	2.56
	$\Gamma=3.1\times10^{-5}$	Eq. (24)	0.6	1.5	0.9	2.4
	$(V=3, J=2)$	Eq. (12)	0.72	1.65	1.19	2.84
HD/Ag	$E_r=83.45\times10^{-5}$	Eq. (20)	0.71	1.65	1.18	2.83
	$\Gamma=2.92\times10^{-5}$	Eq. (24)	0.7	1.6	1.1	2.5
	$(V=4, J=2)$	Eq. (12)	0.665	1.44	0.96	2.40
HD/Ag	$E_r=103.5\times10^{-5}$	Eq. (20)	0.665	1.44	0.96	2.40
	$\Gamma=2.36\times10^{-5}$	Eq. (24)	0.66	1.4	0.9	2.3
	$(V=5, J=2)$	Eq. (12)	0.625	0.99	0.62	1.61
HD/Ag	$E_r=116.9\times10^{-5}$	Eq. (20)	0.625	0.99	0.62	1.61
	$\Gamma=1.55\times10^{-5}$	Eq. (24)	0.61	0.98	0.6	1.58

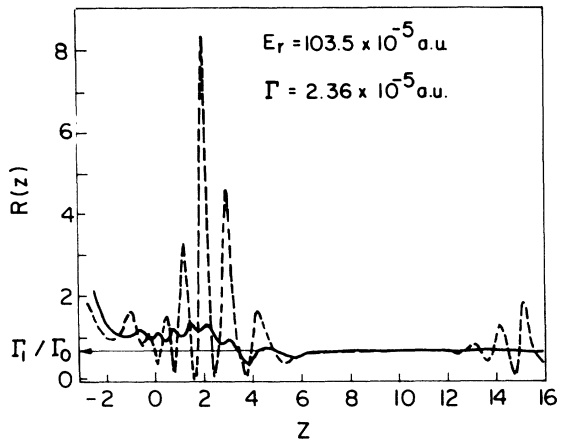

FIG. 2. Comparison between the branching ratios obtained from Eq. (20) (solid line) and Eq. (24) (dashed line) by the asymptotic analysis of the ($V=4$, $J=2$) HD/Ag(111) predesorption resonance, illustrating the enhanced stability of the results obtained from the new formula given in Eq. (20). $R(z)=\Gamma_1(z)/\Gamma_0(z)$ is the local branching ratio as defined in Eqs. (24) and (20), where ∞ is replaced by r.

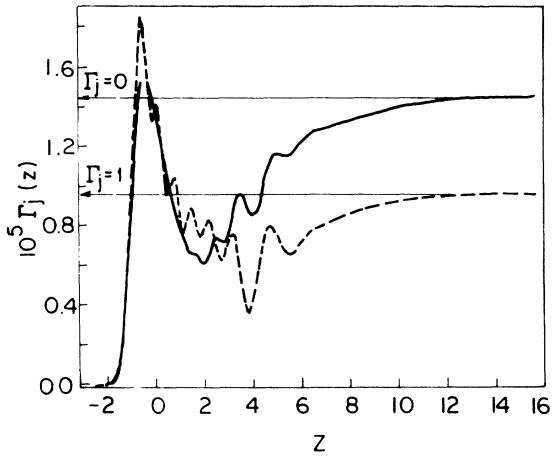

FIG. 3. Partial widths of the ($V=4$, $J=2$) HD/Ag(111) predesorption resonance obtained directly by separate calculations of the denominator $\Gamma_{J=0}(r)$ and the numerator $\Gamma_{J=1}(r)$ of Eq. (20) [with the coefficients from Eq. (19)].

scaling, respectively, r and z by a complex factor $\exp(i\theta)$. The rotational angle θ has been optimized to give a stationary solution in the complex linear variational space, i.e., $dE_r/d\theta=0$, $d\Gamma/d\theta=0$ when E_r and Γ are, respectively, the resonance position and width. The corresponding eigenvector has been used to calculate the branching ratios and the partial widths as given by Eqs. (12), (20) (new formula), and (24). The results presented in Fig. 1 constitute a representative example for the stability of the branching ratios with respect to the variation of the rotational angle θ and the box size L.

The results for the studied multichannel model problems are summarized in Table I. Equation (24) was applied before to these resonances.[6] [However, the results presented here for the HD/Ag(111) predesorption resonances are more stable since we scale Z rather of the box size L, as we did in Ref. 6.] As one can see from Table I the results obtained from the asymptotic analysis of the resonance wave functions Eq. (24), from the new formula given in Eq. (20), and from the integral given in Eq. (12), are consistent and provide a numerical support to our proof given in Sec. II that for an *infinite* number of basis functions Eqs. (12), (20), and (24) are identical and should provide exactly the same values of the partial widths.

The partial widths and the branching ratios were obtained from Eqs. (20) and (24) by the asymptotic analysis of the resonance wave function. The main difference between the two formulas [and also between Eq. (20) and Bačić and Simons formula] in the substitution of the resonance function Φ_J in Eq. (20) by its asymptotical limit, in order to get the formula of Eq. (24), which has been used before. A comparison between the results obtained from Eqs. (20) and (24) (see Fig. 2) clearly show that the new formula for the branching ratio given in Eq. (20) provides a more stable value for the branching ratio of HD/Ag(111) predesorption resonances. The use of formula (20) rather than Eq. (24) not only increases dramatically the stabilization length of the plateau but also reduces the amplitude of the oscillations obtained near the edge of the box. The spurious oscillations in Fig. 2 on the far right apparently come from the presence of the oscillating exponential in Eq. (24).

It is interesting to point out that although Eq. (20) has been derived for the branching ratio (i.e., the ratio between two partial widths), an estimate of the two partial widths can be directly obtained by separate calculations of the denominator and the numerator of Eq. (20) [with the coefficients from Eq. (19)]. An illustrative numerical result showing the stability of the directly obtained particle widths is given in Fig. 3. The results presented in Table I show that the sum of the partial widths, obtained as described above, is very close to the total width given by twice the imaginary part of the complex eigenvalue of the complex scaled Schrödinger equation.

IV. SUMMARY

A complex scaling resonance-scattering theory has been developed here to obtain partial widths and branching ratios for a full scattering experiment. We postulate here that during the full scattering process, for which the dominant intermediate state is the resonant one, the complex "energy" should be conserved. It implies that not only the energy (i.e., the real part of the complex resonance eigenvalue) should be conserved, but also the lifetime of the dissociative event (i.e., the imaginary part of the complex resonance eigenvalue) should remain constant. Equation (20) is a new formula for the branching ratio. The coherent formalism presented here provides a simple relationship between the different procedures for

calculating partial widths proposed by Noro and Taylor, Bačić and Simons, and more recently by Peskin, Moiseyev, and Lefebvre. All formulas of partial widths and branching ratio derived here were checked by calculating the partial widths of two multichannel model Hamiltonians.

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