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Complex Coordinate Rotation Calculation of Branching Ratios

ZLATKO BAČIĆ* AND JACK SIMONS†

Chemistry Department, University of Utah Salt Lake City, Utah 84112, U.S.A.

Abstract

It is shown how branching ratios can be obtained from complex coordinate rotation calculations. The procedure is applied to a rotational Feshbach resonance in a model atom–diatom van der Waals complex which has two open channels present, and to a simple two-channel model potential problem which has been treated by other workers.

1. Introduction

Two methods have recently received much attention for use in direct calculations of energies and widths (or, equivalently, lifetimes) of electron–atom and electron–molecule scattering resonance states; the method of complex coordinate rotation [1] (complex scaling) and the Siegert method [2, 3]. The coordinate rotation (CR) method has, in the past few years, been extensively applied to the study of electron scattering resonances involving atoms and molecules [1]. Very recently, it was also demonstrated that rotational predissociation [4] (in H_2^-) and metastable states of atom–diatom complexes [5, 6] can also be effectively studied by this method. A few calculations using the Siegert method have been performed on several autoionizing states of H^- [3, 7], He [7], and He^- [8].

As is emphasized later in this paper, the CR method permits the straightforward treatment of resonance states which possess N open channels, by the inclusion of appropriate square integrable functions in the basis set. Extension of the Siegert method to many channel problems requires addition of N divergent Siegert-type wave functions to the basis set, each such function corresponding to outgoing flux with kinetic energy appropriate to its channel. Numerical problems associated with the evaluation of the Hamiltonian matrix elements in such a basis set have not been adequately discussed in the literature. Analytic continuation techniques have been successfully employed in the one open channel case and in a "square well" model two channel case [9], but it is not clear how feasible and accurate such calculations would be when one must deal with several Siegert functions having different divergence rates.

Both the CR and Siegert methods calculate the complex resonance eigenvalue, the imaginary part of which gives the total width of the resonance. The question that naturally arises is how to compute the branching ratios (and partial widths)

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* University of Utah Graduate Research Fellow.

† Camille and Henry Dreyfus Fellow; John Simon Guggenheim Fellow.

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given the resonance eigenvalue and the associated CR or Siegert wave function. Expressions for calculating partial widths from Siegert wavefunctions have been derived in two recent papers [9, 10]. Moreover, Noro and Taylor [11] recently demonstrated how one could use the CR wave function, together with appropriately chosen "unperturbed" wave functions (the Φ_β of Ref. 11) to compute branching ratios. It is the purpose of the present paper to demonstrate how the branching ratios can be extracted from CR calculations with little additional effort in a manner which differs from that of Ref. 11 in that no use is made of unperturbed wave functions. The significance of this point is made clear below. We do not intend to make a critical comparison of the Siegert and CR methods. Our primary reason for considering the Siegert method is so that we can use the available expressions for branching ratios in terms of the Siegert wave function together with the connection between Siegert and CR wave functions shown here to obtain branching ratios from CR results.

In Section 2 we show that under certain circumstances, the Siegert and CR resonance wave functions are proportional to one another. We exploit this fact in Section 3 to derive an expression for the branching ratio. In Section 4 we use our method to study two model problems: a rotational Feshbach resonant state in an atom–diatom van der Waals complex with two open channels and a simple two-channel model potential problem previously treated by Noro and Taylor [11]. Section 5 contains some concluding remarks.

2. Relation Between Siegert and CR Wave Functions

Let us consider the scattering of a (distinguishable) particle A at $\mathbf{r}$ by a molecule BC whose internal-state energies and wave functions are denoted by ε_n and $T_n(R)$, and whose internal Hamiltonian is $h_{BC}(R)$. The Schrödinger equation for the composite $A+BC$ system is (μ is the A—BC reduced mass)

$$\left(-\frac{\hbar^2}{2\mu}\nabla_r^2+h_{BC}+V(\mathbf{r},R)-E\right)\psi_s(\mathbf{r},R)=0. \tag{2.1}$$

The wave function ψ_s is, in the Siegert method, expanded in terms of products of target-molecule functions T_n and scattering functions. These scattering functions are expanded in a convenient basis of localized square integrable functions $\{g_j(r)\}$ and, for each *open* channel, an outgoing Siegert function $S_n(r)$. For s-wave scattering, the $S_n(r)$ are usually taken to have the form $(1-e^{-\alpha r})\,e^{ik_nr}/r$, where $(1-e^{-\alpha r})$ is a "cutoff function" used to guarantee proper $r\to 0$ behavior, and $\hbar^2k_n^2/2\mu=E-\varepsilon_n$. When such an expansion

$$\psi_s=\sum_{nj}T_ng_jB_{nj}+\sum_{n(\text{open})}A_nT_nS_n \tag{2.2}$$

is used in Eq. (2.1), premultiplication by $T_mg_{j'}$ and T_mS_m, and integration over $\mathbf{r}$ and R leads to a (non-Hermitian) eigenvalue problem for the resonance energy E and the expansion coefficients B_{nj} and A_n. This eigenvalue problem must be solved iteratively since the energy E appears in the expression which defines the Siegert functions' wave vectors k_n. Upon convergence, one eigenvalue E of the secular problem may be consistent with the E used to define the k_n. This is the desired (complex) resonance energy E_c.

We may alternatively calculate the resonance energy (its position and width) by using the coordinate rotation method. Under the well known transformation (which is applied only to that coordinate which lies in the continuum)

$$\mathbf{r} \to \mathbf{r}\, e^{i\theta}. \tag{2.3}$$

The Schrödinger equation (2.1) becomes

$$\left(-\frac{\hbar^2}{2\mu} e^{-2i\theta}\, \nabla_r^2 + V(\mathbf{r}\, e^{i\theta}, R) + h_{BC} - E(\theta)\right)\psi_\theta(\mathbf{r}, R) = 0. \tag{2.4}$$

It has been shown that if the rotation angle θ is taken large enough (but $<\frac{1}{2}\pi$), the desired resonance eigenvalue of Eq. (2.4) will become θ independent. Hence by computing the eigenenergies of Eq. (2.4), or some approximation to the same, as θ is increased, one should be able to identify the resonance eigenvalue as that one which becomes independent of (or at least slowly varying with)θ for θ beyond some critical angle. Upon the expansion of ψ_θ in a finite square integrable (without Siegert continuum functions) basis set, the desired complex resonance eigenvalue (E_{CR}) can be found by the above outlined process and is given by

$$E_{\mathrm{CR}} = E_r - i(\Gamma/2), \tag{2.5}$$

where E_r and Γ represent the position and width of the resonance state, respectively. The resonance eigenfunction $\psi_\theta(r)$ is square integrable and vanishes at the origin. The "critical" value of the transformation angle θ at which the resonance eigenvalue becomes invariant (or relatively stable) with respect to further increases of θ, will be denoted as θ_c.

In contrast to the square integrable nature of the CR wave function the Siegert function is divergent for $r \to \infty$ since each of the wave vectors k_n has negative imaginary part (since E_c does)

$$k_n = |k_n|\, e^{-i\beta_n}, \tag{2.6}$$

where

$$|k_n| = \sqrt{2}\,[(E_r - \varepsilon_n)^2 + \Gamma^2/4]^{1/4} \tag{2.7}$$

and

$$\beta_n = \tfrac{1}{2}\tan^{-1}\left(\frac{\Gamma/2}{E_r - \varepsilon_n}\right). \tag{2.8}$$

To achieve any connection between the Siegert state and $\psi_\theta(\mathbf{r}, R)$ it is, of course, necessary to remove the divergent nature of the Siegert wave function.

If the Siegert expansion given in Eq. (2.2) is evaluated at $\mathbf{r}\, e^{i\theta}$, the asymptotic ($r \to \infty$) pieces become (for s-wave scattering)

$$A_n T_n S_n(\mathbf{r}\, e^{i\theta}) = e^{-i\theta} A_n T_n r^{-1} \exp\left[i|k_n| r \cos(\theta - \beta_n) - |k_n| r \sin(\theta - \beta_n)\right], \tag{2.9}$$

which is square integrable if $\theta > \beta_n$. With this hint at how to make the desired wave function connection, we can evaluate Eq. (2.1) (the equation obeyed by ψ_s) at $\mathbf{r}\, e^{i\theta}$ and use

$$\frac{d}{d(r\, e^{i\theta})} = e^{-i\theta} \frac{d}{dr} \tag{2.10}$$

to write

$$\left(-\frac{\hbar^2}{2\mu} e^{-2i\theta}\, \nabla_r^2 + V(\mathbf{r}\, e^{i\theta}, R) + h_{BC} - E \right) \psi_s(\mathbf{r}\, e^{i\theta}) = 0. \tag{2.11}$$

The rotated Siegert wave function $\psi_s(\mathbf{r}\, e^{i\theta})$, thus obeys the same equation [Eq. (2.11) or Eq. (2.4)] and boundary conditions as $\psi_\theta(\mathbf{r})$ for $\theta > \max(\beta_n)$, since for these θ's, the most divergent component of ψ_s has been made square integrable (just as ψ_θ) and, for $\theta > \max(\beta_n)$, ψ_θ has a θ-independent eigenenergy

$$E(\theta) = E_c = E_r - i\Gamma/2. \tag{2.12}$$

Thus, when $\theta > \max(\beta_n)$, $\psi_s(\mathbf{r}\, e^{i\theta})$, and $\psi_\theta(\mathbf{r})$ satisfy identical second order differential equations and obey the same boundary conditions at $r = 0$ and $r \to \infty$. We therefore conclude that the two functions are proportinal to one another, i.e.,

$$\psi_s(\mathbf{r}\, e^{i\theta}) = K\psi_\theta(\mathbf{r}) \quad \text{for } \theta > \max(\beta_n). \tag{2.13}$$

We emphasize that the above proportionality holds only when $\theta > \max(\beta_n)$. For $\theta \le \max(\beta_n)$, $\psi_s(\mathbf{r}\, e^{i\theta})$ does not belong to the class of square integrable functions. Hence, it cannot be compared to $\psi_\theta(\mathbf{r})$. In addition, for $\theta \le \max(\beta_n)$, Eqs. (2.4) and (2.11) are not identical since for these angles, $E(\theta)$ in Eq. (2.4) does depend on θ. Let us now explore the proportionality between $\psi_s(\mathbf{r}\, e^{i\theta})$ and $\psi_\theta(\mathbf{r})$ to achieve the desired branching ratio result.

3. Evaluation of Branching Ratios

For the purpose of deriving a branching ratio expression we assume that, for an atom–diatom scattering problem, a resonance state has been located and its position and width calculated (via both the Siegert and CR methods). The resultant CR resonance wave function can be written in the square integrable basis $\{g_l\}$ as

$$\psi_\theta(\mathbf{r}) = \sum_n \sum_l C_{nl}(\theta) T_n g_l(r). \tag{3.1}$$

The Siegert wave function for the same resonance state, evaluated at $\mathbf{r}\, e^{i\theta}$, is

$$\psi_s(\mathbf{r}\, e^{i\theta}) = \sum_n \sum_l B_{nl} T_n g_l(\mathbf{r}\, e^{i\theta}) + \sum_{n(\text{open})} A_n T_n S_n(\mathbf{r}\, e^{i\theta}). \tag{3.2}$$

In both Eqs. (3.1) and (3.2), the T_n's are target-molecule wave functions and the g_l's are localized square integrable wave functions, just as in Eq. (2.2).

As was shown in Section 2 [Eq. (2.13)], $\psi_\theta(\mathbf{r})$ and $\psi_s(\mathbf{r}\, e^{i\theta})$ are proportional to one another for $\theta > \max(\beta_n)$. Projecting both sides of Eq. (2.13) onto a particular target state T_m, we obtain

$$\sum_j B_{mj} g_j(\mathbf{r}\, e^{i\theta}) + A_m S_m(\mathbf{r}\, e^{i\theta}) = K \sum_l C_{ml}(\theta) g_l(r). \tag{3.3}$$

The first term (i.e., the summation) on the left-hand side of Eq. (3.3) consists of a sum of localized exponentially decaying functions. It describes the resonance state in the region where atom–diatom interaction is significant (i.e., the nonasymptotic region). We assume that this region can be bounded by a sphere with radius $R = L$, beyond which the potential interaction is essentially zero and the localized wave function amplitude is vanishingly small. This implies that

$$B_{mj} g_j(\mathbf{r}\, e^{i\theta}) = 0 \quad \text{for } r > L. \tag{3.4}$$

The optimal choice of L is discussed below, when we come to apply the results obtained here to a model atom–diatom scattering problem. Under this assumption, Eq. (3.3) becomes (using the explicit form of the Siegert continuum functions S_n)

$$A_m \frac{e^{i|k_m| r e^{i(\theta - \beta_m)}}}{r e^{i\theta}} = K \sum_l C_{ml}(\theta) g_l(r|r > L) \quad \text{for } r > L. \tag{3.5}$$

The symbol $g(r|r > L)$ in Eq. (3.5) means that the argument r is to be restricted to the region $r > L$. The rotated cutoff function $f(r\, e^{i\theta}) = (1 - e^{-\alpha r e^{i\theta}})$ is omitted from the left-hand side of Eq. (3.5), since for $r > L$, $f(r\, e^{i\theta}) \approx 1$. After slightly rearranging Eq. (3.5) and integrating both sides of the equation over r, from L to infinity [keeping in mind that $\exp(i|k_m| r\, e^{i(\theta - \beta_m)}) \to 0$ as $r \to \infty$ for $\theta > \beta_m$], we arrive at the following expression for A_m:

$$A_m = -K\, e^{i\theta}\, i|k_m| e^{(i(\theta - \beta_m)} e^{-i|k_m| L e^{i(\theta - \beta_m)}} \sum_l C_{ml}(\theta) \int_L^\infty g_l(r) r\, dr. \tag{3.6}$$

Calculation of branching ratios requires the amplitude $|A_m|^2$, which is given by

$$|A_m|^2 = K^2 |k_m|^2\, e^{2|k_m| L \sin(\theta - \beta_m)} \left| \sum_l C_{ml}(\theta) \int_L^\infty g_l(r) r\, dr \right|^2. \tag{3.7}$$

Then, the branching ratio for any pair of open channels is given by

$$\left| \frac{A_m}{A_p} \right|^2 = \left| \frac{k_m}{k_p} \right|^2 \frac{e^{2|k_m| L \sin(\theta - \beta_m)}}{e^{2|k_p| L \sin(\theta - \beta_p)}} \left| \frac{\sum_l C_{ml}(\theta) \int_L^\infty g_l(r) r\, dr}{\sum_l C_{pl}(\theta) \int_L^\infty g_l(r) r\, dr} \right|^2. \tag{3.8}$$

This result, when evaluated at the value of θ [$\theta = \max(\beta_n)$], represents our technique for evaluating the branching ratio for open channels m and p.

In the limit of a narrow resonance, for which the width Γ is smaller than the spacings between the target's internal energy levels (the thresholds), the partial scattering width Γ_m can be interpreted as the decay rate of the metastable state into the open channel m [10]. In this case, the ratio of partial widths for any two open channels can be calculated using the branching ratio expression, Eq. (3.8):

$$\Gamma_m/\Gamma_p = |A_m/A_p|^2. \tag{3.9}$$

If the A_m's are normalized so as to require

$$\sum_{m=1}^{N} |A_m|^2 = 1, \tag{3.10}$$

the partial widths sum (for the case of a narrow resonance) to the total width Γ:

$$\Gamma = \sum_n \Gamma_n. \tag{3.11}$$

Thus, the coordinate rotation method allows us to determine the total width and all of the partial widths, using Eqs. (2.5) and (3.9), respectively.

Our branching ratio expression, Eq. (3.8), contains the parameter L, the practical choice of which remains to be discussed. However, it does not contain reference to an "unperturbed" scattering wavefunction such as appears in Ref. 11. We do need to know what the *asymptotic* form of the Siegert function is in each channel, but we do not have to separately solve a scattering problem (with the interchannel coupling turned off) to obtain unperturbed functions. It is quite clear from the discussion preceding Eq. (3.4) that the value of L should be sufficiently large that it falls outside the region where the atom–diatom interaction is appreciable. In CR calculations on atom–diatom collision complexes [5, 6], as mentioned briefly in Section 2, the radial wave function is expanded in terms of square integrable basis functions. Our own CR calculations [12] show that increasing the size of the basis set (adding L^2 functions capable of describing the atom–diatom translational motion at larger and larger r, beyond the "range" of the potential interaction) results in a resonance eigenvalue that is "stable" in the sense that it is insensitive to further addition of basis functions. As Hazi and Taylor [13] demonstrated long ago, square integrable basis sets are capable of describing the resonance wave function both in the strong interaction region and in regions where $V \approx 0$ (if the basis extends to these regions). We have indeed observed [12] in plotting the r dependence of our open-channel wave functions that a damped sinusoidally oscillating function of the correct de Broglie wavelength can be obtained within our basis sets. Clearly, L should be chosen so as to lie in this "region of stability" beyond which ($r > L$) addition of radial basis functions does not change the resonance eigenvalue. In this region "beyond" the atom–diatom potential well, the resonance eigenfunction has the "asymptotic" form given in Eq. (3.5). Hence by using Eq. (3.8), we can calculate the branching ratio. We would not expect the calculated branching ratios to be very sensitive to the choice of L, as long as L lies in the asymptotic region described above. Of course, for practical reasons, one hopes to choose L to have it in the asymptotic region, yet to have L small enough that a reasonably small number of square integrable basis functions $\{g_l\}$ can be used to span the space $r \leq L$.

4. Model Problems

A. *Atom–Diatom Rotational Feshbach Resonance*

The CR procedure developed in Sections 2 and 3 is applied here to a model van der Waals atom–diatom A–BC system which has two open channels present. The Hamiltonian for this system is

$$H(\mathbf{R}, \mathbf{r}, \theta) = -\frac{\hbar^2}{2\mu}\left[\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right) - \frac{l^2}{r^2}\right] + B_d j^2 + V(r, \theta), \tag{4.1}$$

where μ is the reduced mass of the system $[m_A m_{BC}/(m_A + m_{BC})]$; θ is the angle between the diatom orientation vector $\mathbf{R}$ and the atom–diatom separation vector $\mathbf{r}$; l^2 is the square of the angular momentum operator associated with rotation of A about BC; j^2 is the square of the angular momentum operator associated with rotation of BC; and B_d is the rotational constant for BC, treated as a rigid rotor. The interaction potential used in this study is taken to be a sum of Lennard-Jones functions having various angular dependances

$$V(r, \theta) = V_0(r) + V_2(r)P_2(\cos\theta), \tag{4.2}$$

where

$$V_0(r) = 4\varepsilon[(\sigma/r)^{12} - (\sigma/r)^6] \tag{4.3}$$

and

$$V_2(r) = 4\varepsilon[b(\sigma/r)^{12} - a(\sigma/r)^6]. \tag{4.4}$$

The values of all of the parameters necessary to specify the model are given in Table I. Rotational Feshbach resonances involving *one* open channel were previously treated for this model problem by the authors [5] and by Chu [6] employing the CR method, and by Grabenstetler and LeRoy [14] using a more conventional scattering approach. A metastable state correlating with the isotropic closed channel $(j = l = 2, J = 0)$ was considered [5, 6, 14]. The quantum numbers j and l refer to the rotation of $\mathbf{R}$ and $\mathbf{r}$, respectively, and J refers to the total angular momentum. The angular basis used in these studies was restricted to

TABLE I. Parameters characterizing the model system.

μ(amu)	1.981
B_d(cm^{-1})	60.551
ε(cm^{-1})	60.408
σ(Å)	3.4745
a	0.09
b	0.5

l, $j \leq 2$ and $J = M = 0$. Thus, only a single open channel ($j = l = 0$, $J = 0$) was allowed.

In the present work $j = 0$, $j = 2$, and $j = 4$ states of the rotor are incluced in the basis and the total angular momentum is restricted to $J = 0$. Hence, *two* open channels, ($j = l = 2, J = 0$) and ($j = l = 0, J = 0$) are available. To expand the radial wave function we used sets of M Gaussian basis functions ($M = 12, 15, 18, 25$). Then, by using the coordinate rotation technique (as described in detail in our earlier paper, Ref. 5) we determined the resonance (complex) eigenvalue associated with the closed channel ($j = l = 4$, $J = 0$) for each of the basis sets. A portion, greatly enlarged to emphasize the behavior near the stable point, of the optimal θ trajectory (for the large $M = 25$ basis) belonging to the resonance eigenvalue is shown in Figure 1. The Gaussian basis functions used in this basis have exponents $\alpha = 39.86$ and centers (in Å) given by $r_l = 3.3 + (l-1) \times 0.264$ ($1 \leq l \leq 25$).

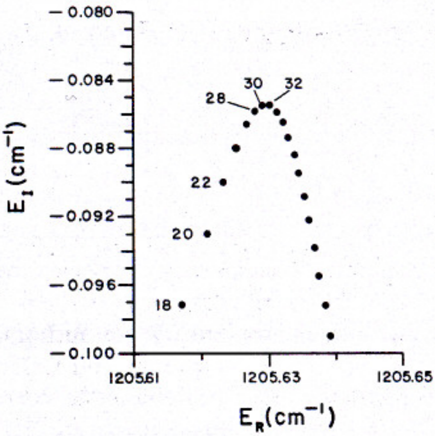

Figure 1. Segment of the θ trajectory of the resonance eigenvalue associated with the metastable level ($j = l = 4, J = 0$) of the model atom–diatom van der Waals system ($M = 25$). The θ increment is 2×10^{-4} rad. The numbers show the rotational angles $\theta \times 10^4$.

It is easily determined from the θ trajectory (Fig. 1) that the resonance energy is 1205.63 cm^{-1}. The width $\Gamma(= -2\,\text{Im}\,E)$ is 0.171 cm^{-1}. Essentially the same results were obtained for the smaller $M = 15, 18$ basis sets. Because the center of the eighteenth Gaussian basis function occurs at $r_{18} = 7.8$ Å, and in view of our discussion in Section 3 regarding the choice of L, it seems to be appropriate to use values of L larger than 7.8 Å in computing the branching ratio via Eq. (3.8). A series of branching ratios $|A_2|^2/|A_0|^2$ computed for various values of L is given in Table II. It is immediately apparent that for $L > 9.5$ Å the branching ratio becomes constant to the extent that it is essentially independent of the choice of L.

TABLE II. Branching ratios for the atom–diatom problem calculated using Eq. (3.8).

L(Å)	$\|A_2/A_0\|^2$
8.40	1.9253
8.60	3.6760×10^3
8.80	6.9039×10^2
9.00	3.0094×10^1
9.20	5.9606×10^1
9.40	1.2354×10^3
9.50	3.7135×10^2
9.55	3.2992×10^2
9.60	3.1304×10^2
9.65	3.0577×10^2
9.70	3.0260×10^2
9.75	3.0118×10^2
9.80	3.0051×10^2
9.85	3.0013×10^2
9.90	2.9987×10^2
9.95	2.9966×10^2
10.00	2.9946×10^2
10.05	2.9927×10^2
10.10	2.9909×10^2
10.15	2.9890×10^2

The value of the branching ratio can, quite unambiguously, be determined to be 3.0×10^2.

B. A Model Two-Channel Potential Problem

Noro and Taylor [11] (NT) demonstrated their procedure for obtaining branching ratios from CR calculations on a model two-channel potential problem; comparison with their results therefore provides a more direct test of our method.

The radial Hamiltonian for the NT model problem is [11] (for *s* wave, in atomic units)

$$H = -\frac{1}{2}\frac{d^2}{dr^2} + H_0(x) + V(x, r), \tag{4.5}$$

where H_0 is a target Hamiltonian defined to have two eigenstates

$$H_0(x)\phi_\alpha(x) = E_\alpha \phi_\alpha(x), \qquad \alpha = 1, 2. \tag{4.6}$$

The matrix elements of the interaction potential between target eigenstates are defined as follows [11]:

$$U_{\alpha\beta}(r) = \int dx\, \phi_\alpha^*(x) V(x, r) \phi_\beta(x) = U_{\alpha\beta} r^2 e^{-r},$$

$$\mathbf{U} = \begin{pmatrix} -1.0 & -7.5 \\ -7.5 & 7.5 \end{pmatrix}. \tag{4.7}$$

The energies of the target states are 0.0 and 0.1. A Slater-type orbital basis set was chosen [11] for expansion of the r dependence of the CR wave function

$$\left.\psi_\theta(x, r) = \sum_{\alpha j} C_j^\alpha(x) r^j e^{-\xi r}\right\} \quad \begin{array}{l} \alpha = 1, 2, \\ j = 1, 2, \ldots, 18, \end{array} \tag{4.8}$$

with the orbital scaling parameter $\xi = 4.0$. The resulting θ trajectory is shown in Figure 2, where we see that, for θ greater than 0.14 rad, E_{CR} becomes essentially independent of the rotation angle. The value of E_{CR} at this stable point is the same as that obtained in Ref. 11 (see Table III).

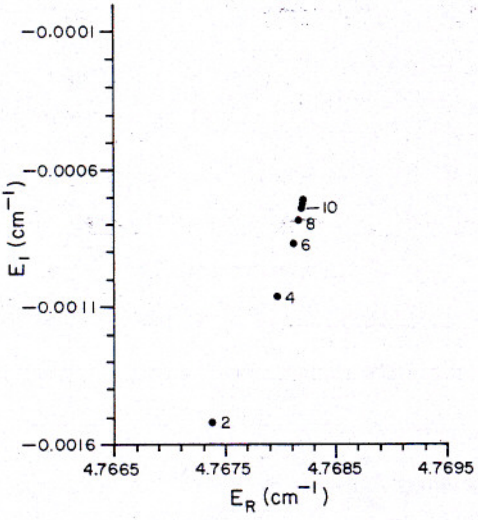

Figure 2. θ Trajectory of the resonance eigenvalue of the two-channel model potential problem. The θ increment is 2×10^{-2} rad. The numbers show the rotational angles $\theta \times 10^2$. Individual trajectory points cannot be resolved on this scale, for $\theta >$ ca. 0.14 rad.

We also found that the branching ratios computed via Eq. (3.8) depend very little on the choice of the parameter L, provided that L is greater than ca. 8 Å {one can see from the paper of NT [11] (Fig. 1) that the two-channel model potential is practically zero for r beyond 8 Å}. However, we find that the branching ratios do exhibit θ dependence which, over a certain range of angles, is rather mild (up to $\theta = 0.26$ rad, see Table IV). The resultant values of the partial widths Γ_1 and Γ_2 calculated on the basis of these branching ratios are given in Table III, together

TABLE III Two-channel model potential results.

	This work	CCR results of NT[11]	Numerical results of NT[11]
E_r	4.7682	4.7682	4.7682
Γ	0.001420	0.001420	0.001421
Γ_1	0.000020[a]	0.000059	0.000061
Γ_2	0.001400[a]	0.001361	0.001360

[a] Obtained at $\theta = 0.24$ rad (see Table IV).

with the results of Noro and Taylor [11]. Because the branching ratio is so small, Γ_1 and Γ_2 must be determined to very high precision (ca. 1%) in order to guarantee that Γ_1/Γ_2 is significant. It can be seen from Figure 2 of Ref. 11 that the NT values of Γ_1/Γ_2 obtained via the CR method range from 0.04 to ca. 0.05 for values of θ near the "stationary point." Our values of Γ_1/Γ_2, up to $\theta = 0.26$ rad (beyond which, for reasons apparent from Table IV, one can have no confidence in the branching ratio results) vary from 0.012 to 0.014 as theta waivers around our stationary point. In fact, it is quite impressive that the two distinct methods, employed by NT [11] and in the present work, are able to obtain branching ratios within a factor of 3 for this difficult case where Γ_1 is only a few percent of Γ_2. We feel that the level of agreement is satisfactory. Moreover, we find it interesting that

TABLE IV. Branching ratios for two-channel model potential

θ/rad	Γ_1/Γ_2[a]
.18	0.0121
.20	0.0130
.22	0.0139
.24	0.0141
.26	0.0143
.28	0.0170
.30	0.0154
.32	0.0128
.34	0.0102
.36	0.0236

[a] Calculated using Eq. (3.8).

a technique which is based upon looking at the *large-r* behavior of the rotated wave function (ours) agrees quite well with one (NT) which emphasizes the *small-r* (interaction region) behavior of the rotated wavefunction. In both methods, it is difficult to obtain a value for Γ_1/Γ_2 which is highly insensitive to theta (partly because Γ_1 is so much smaller than Γ_2); these difficulties are emphasized in Figure 2 of Ref. 11 and in our Table IV. This fact makes a highly critical comparison of the two methods rather difficult. It would be useful to find a model problem for which Γ_1/Γ_2 is of the order of 0.1 which would make such a comparison easier.

5. Concluding Remarks

The fact that we choose to examine the large-r behavior of the CR wave function is, in a sense, what distinguishes our approach from that of Ref. 11 where the small-r (strong interaction) region is emphasized. The price which we pay in attempting to extract the branching ratios from the asymptotic behavior of ψ_θ is that we have to have a large enough r basis to accurately extend beyond the "range" of V. By concentrating on the small-r region, the workers of Ref. 11 avoid this basis set problem. However, in return, they must know more than just the asymptotic form of the open channel decay states; they have to compute *separately* the full (asymptotic and small-r) scattering state which describes the A–to–BC relative motions in the *absence* of interchannel couplings. We avoid such "unperturbed" calculations. For problems involving interactions among several indistinguishable particles (e.g., electronic Feshbach resonances), it is not entirely clear how one should best go about computing the "unperturbed" open-channel functions needed in Ref. 11. To "turn off" the coupling which gives rise to the metastable state is more difficult there, especially if one is using a multiconfigurational wave function to describe the resonance state. We therefore feel that further investigations of the kinds of branching ratio formulas given here and in Ref. 11 are necessary if we are to gain understanding of how to best evaluate resonance-state properties.

Clearly, further numerical experience is required before we can make more definitive statements about the range of applicability of our branching ratio expression. The two open channel rotational Feshbach resonance problem treated here represents the first application of our results to a full three dimensional scattering problem. It is our plan for the immediate future to apply the several open channel CR methods as described here to vibration–rotation Feshbach resonances involving van der Waals complexes such as HeI_2. Our desire is to explore the range of utility of the method and to then carry out model studies for van der Waals complexes which are of current experimental interest.

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