Addendum to "Direct trajectory method for semiclassical wave functions"

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(Received 13 May 2001; revised manuscript received 29 August 2001; published 5 February 2002)

For two kinetically coupled Morse oscillators, we present details of the method of calculation in Ref. [1] of the semiclassical wave function for an Einstein-Brillouin-Keller quantizing torus, using a single trajectory and its stability matrix. This is the "standard" method, contrasted in Ref. [1] with our new "direct" method, which does not require the calculation of the stability matrix.

DOI: 10.1103/PhysRevA.65.034103 PACS number(s): 03.65.Sq

I. INTRODUCTION

In Ref. [1], we tested a new method for semiclassical wave functions corresponding to an invariant tori satisfying Einstein-Brillouin-Keller (EBK) quantization conditions. This "direct" method is intuitively very appealing; one simply attaches a semiclassical wave to a trajectory on the quantizing torus, and lets the trajectory run, building the phase-coherent wave function. The semiclassical amplitude is taken simply as the numerically accumulated classical density. This avoids the need to deal with the cumbersome stability matrix in the usual implementations of the EBK wave function method. We compared our direct method with the "standard" method of Maslov and Fedoriuk [2], and found that they give identical results within numerical accuracy, as demonstrated in Fig. 2 of Ref. [1].

In this Addendum, we present details, omitted in Ref. [1], of our computational implementation of the standard method of Maslov and Fedoriuk. We plan in a later paper to compare for *chaotic* systems the results of the direct and standard methods, applied to *cantori*, the remnants of tori broken up by chaos. It, therefore, seems advisable in this Addendum to explain the rather involved details of our implementation of the standard method. Furthermore, there actually are very few demonstrations of the EBK wave-function method. One is the calculation of Knudson *et al.* [3] on coupled oscillators. Their computational method differs in certain respects from ours. For this reason as well, it seems worthwhile to spell out exactly what we did in Ref. [1].

The "EBK quantization conditions" were postulated by Einstein [4] in 1917, together with the conjectured existence of invariant tori in the classical mechanics of nonintegrable systems. The formalism for the semiclassical wave function corresponding to an EBK torus was not developed until 1958 by Keller [5]. Still later, Maslov and Fedoriuk [2] developed a theory for the semiclassical wave function. The difference between these two theories is the use of local coordinates in the former and global coordinates in the latter in the representation of the amplitude factor.

Knudson *et al.* [3] successfully applied the Maslov-Fedoriuk formalism to the regular region of a system of two coupled harmonic oscillators. Our implementation in Ref. [1] of the "standard" Maslov-Fedoriuk method is different from theirs. They used one trajectory to get the phase factor, and two others to get the amplitude factor, determining the influence of the stability by observing numerically the divergence of two distinct trajectories. We do the entire calculation by running one trajectory. Like Knudson *et al.*, we get the phase by attaching a semiclassical wave to the trajectory. However, we calculate the amplitude by simultaneously solving the equations of motion and the stability equations for our single trajectory.

II. COUPLED MORSE OSCILLATOR SYSTEM

The system of two kinetically coupled Morse oscillators has been studied by several workers [6–8] as a model for the stretch motions of a polyatomic molecule such as H_2O. Its Hamiltonian is given by

$$H=\frac{p_1^2}{2m}+D(1-e^{-\beta x_1})^2+\frac{p_2^2}{2m}+D(1-e^{-\beta x_2})^2+\alpha p_1 p_2, \tag{1}$$

which can be scaled to the form

$$\varepsilon=\tilde{p}_1^2/2+(1-e^{-\tilde{x}_1})^2+\tilde{p}_2^2/2+(1-e^{-\tilde{x}_2})^2+\delta\tilde{p}_1\tilde{p}_2 \tag{2}$$

by the transformations

$$\varepsilon=H/D,\ \ \tilde{p}_i=(1/\sqrt{mD})\,p_i,\ \ \tilde{x}_i=\beta x_i,\ \ \tau=D\gamma t, \tag{3}$$

where

$$\delta=m\alpha=(m/M)\cos\theta \tag{4}$$

is the coupling constant related to the finite mass M of the central atom, m is the reduced mass of the light atom and the heavy central atom, θ is the angle made by the two bonds of the molecule, D is the dissociation energy of the Morse oscillator, β is the Morse parameter of the system, and $\gamma=\omega_0/\sqrt{2}D$, with $\omega_0=\sqrt{2\beta^2D/m}$ the small oscillation frequency of the Morse oscillator.

III. SEMICLASSICAL WAVE FUNCTION OF AN EBK-QUANTIZING TORUS

A two degree-of-freedom invariant torus is quantized if it satisfies EBK quantization conditions:

$$\begin{aligned}\oint_{C_\alpha}(\tilde{p}_1 d\tilde{x}_1+\tilde{p}_2 d\tilde{x}_2)&=2\pi\hbar\gamma(n_\alpha+\tfrac{1}{2}),\\ \oint_{C_\beta}(\tilde{p}_1 d\tilde{x}_1+\tilde{p}_2 d\tilde{x}_2)&=2\pi\hbar\gamma(n_\beta+\tfrac{1}{2}),\end{aligned} \tag{5}$$

where C_α and C_β are independent circuits, n_α and n_β are integers, $\tilde{x}_1,\tilde{x}_2,\tilde{p}_1,\tilde{p}_2$ are dimensionless coordinates and momenta, and γ is the constant related to the scaling transformation in the previous section. The semiclassical wave function for the torus can be written as [2]

$$\psi(\tilde{x}_1,\tilde{x}_2,\varepsilon)=\sum_{r=1}^{n}\sqrt{\left|\frac{J_r(0,\tilde{x}_{20})}{J_r(\tau,\tilde{x}_{20})}\right|}\exp\left[\frac{i}{\hbar\gamma}S_r(\tau,\tilde{x}_1,\tilde{x}_2)-i\frac{\mu_r(\tau)\pi}{2}\right], \tag{6}$$

where $S_r(\tau,\tilde{x}_1,\tilde{x}_2)=\int_0^\tau(\tilde{p}_1\dot{\tilde{x}}_1+\tilde{p}_2\dot{\tilde{x}}_2)dt$ is the phase along a classical trajectory. The Maslov index $\mu_r(\tau)$ is the number of times that the trajectory has passed through classical caustics, or turning points, at time τ. The subscript r means at time τ the trajectory is in the rth "branch" [3]; for the coupled oscillator system the number of branches is $n=4$.

In Eq. (6) no initial distribution appears, in contrast to Ref. [2]. The reason for this is that we will obtain the wave function by running a *single* classical trajectory.

The Jacobian determinant J_r in Eq. (6) is related to the divergence of nearby trajectories and is given by

$$J_r(\tau,\tilde{x}_{20})=\det\frac{\partial(\tilde{x}_1,\tilde{x}_2)}{\partial(\tau,\tilde{x}_{20})}=\dot{\tilde{x}}_1\frac{\partial\tilde{x}_2}{\partial\tilde{x}_{20}}-\dot{\tilde{x}}_2\frac{\partial\tilde{x}_1}{\partial\tilde{x}_{20}}, \tag{7}$$

where it is understood that $\tilde{x}_{20}$, τ are fixed when we take the partial derivatives. The choice $\tilde{x}_{20}$ for the direction in which to take the partial derivatives is arbitrary [2]. J_r can be negative; its absolute value is proportional to the inverse of the classical density for the trajectory. The partial derivatives in Eq. (7) relate to the stability of the classical trajectory, which will be determined by stability equations in Sec. IV. The Jacobian determinant J_r is zero at the classical turning point. There, Eq. (6) diverges, so the semiclassical wave function is a "primitive" type.

$J_r(0,\tilde{x}_{20})$ appears in Eq. (6) as the initial value of the Jacobian determinant, and from Eq. (7), is given by

$$J_r(0,\tilde{x}_{20})=\left[\det\frac{\partial(\tilde{x}_1,\tilde{x}_2)}{\partial(\tau,\tilde{x}_{20})}\right]_{\tau=0}=\dot{\tilde{x}}_{10}, \tag{8}$$

i.e., the $\tilde{x}_1$ component of the initial velocity of the classical trajectory.

IV. DETERMINATION OF THE JACOBIAN DETERMINANT

In this section we outline in detail the most difficult part of the numerical execution of the semiclassical wave-function method, the calculation of the Jacobian determinant. Our development in part follows loosely the treatment of Greene [9] for a classical map.

As stated earlier, we build the wave function by running just a single, arbitrary trajectory on the invariant EBK torus; we can do this because, in general, such a trajectory will-densely cover the torus. The time evolution of the trajectory is governed by the Hamiltonian equations of motion

$$\frac{d}{d\tau}\begin{bmatrix}\tilde{x}_1\\ \tilde{p}_1\\ \tilde{x}_2\\ \tilde{p}_2\end{bmatrix}=\begin{bmatrix}\dfrac{\partial\varepsilon}{\partial\tilde{p}_1}\\ -\dfrac{\partial\varepsilon}{\partial\tilde{x}_1}\\ \dfrac{\partial\varepsilon}{\partial\tilde{p}_2}\\ -\dfrac{\partial\varepsilon}{\partial\tilde{x}_2}\end{bmatrix}. \tag{9}$$

Now consider a nearby trajectory. Its displacement from the first is denoted as

$$\Delta Z=\begin{bmatrix}\Delta\tilde{x}_1\\ \Delta\tilde{p}_1\\ \Delta\tilde{x}_2\\ \Delta\tilde{p}_2\end{bmatrix}. \tag{10}$$

ΔZ evolves with time τ. The equations that determine $\Delta Z(\tau)$ are obtained by taking the difference in both sides of Eq. (9):

$$\frac{d}{d\tau}\begin{bmatrix}\Delta\tilde{x}_1\\ \Delta\tilde{p}_1\\ \Delta\tilde{x}_2\\ \Delta\tilde{p}_2\end{bmatrix}=\begin{bmatrix}\Delta\dfrac{\partial\varepsilon}{\partial\tilde{p}_1}\\ -\Delta\dfrac{\partial\varepsilon}{\partial\tilde{x}_1}\\ \Delta\dfrac{\partial\varepsilon}{\partial\tilde{p}_2}\\ -\Delta\dfrac{\partial\varepsilon}{\partial\tilde{x}_2}\end{bmatrix}. \tag{11}$$

Note that ε and its partial derivatives are functions of $\tilde{x}_1$, $\tilde{p}_1$, $\tilde{x}_2$, and $\tilde{p}_2$. Taking the first-order difference, we get

$$\frac{d}{d\tau}\begin{bmatrix}\Delta\tilde{x}_1\\ \Delta\tilde{p}_1\\ \Delta\tilde{x}_2\\ \Delta\tilde{p}_2\end{bmatrix}=\underbrace{\begin{bmatrix}\dfrac{\partial^2\varepsilon}{\partial\tilde{x}_1\partial\tilde{p}_1} & \dfrac{\partial^2\varepsilon}{\partial\tilde{p}_1^2} & \dfrac{\partial^2\varepsilon}{\partial\tilde{p}_1\partial\tilde{x}_2} & \dfrac{\partial^2\varepsilon}{\partial\tilde{p}_1\partial\tilde{p}_2}\\ -\dfrac{\partial^2\varepsilon}{\partial\tilde{x}_1^2} & -\dfrac{\partial^2\varepsilon}{\partial\tilde{x}_1\partial\tilde{p}_1} & -\dfrac{\partial^2\varepsilon}{\partial\tilde{x}_1\partial\tilde{x}_2} & -\dfrac{\partial^2\varepsilon}{\partial\tilde{x}_1\partial\tilde{p}_2}\\ \dfrac{\partial^2\varepsilon}{\partial\tilde{x}_1\partial\tilde{p}_2} & \dfrac{\partial^2\varepsilon}{\partial\tilde{p}_1\partial\tilde{p}_2} & \dfrac{\partial^2\varepsilon}{\partial\tilde{x}_2\partial\tilde{p}_2} & \dfrac{\partial^2\varepsilon}{\partial\tilde{p}_2^2}\\ -\dfrac{\partial^2\varepsilon}{\partial\tilde{x}_1\partial\tilde{x}_2} & -\dfrac{\partial^2\varepsilon}{\partial\tilde{p}_1\partial\tilde{x}_2} & -\dfrac{\partial^2\varepsilon}{\partial\tilde{x}_2^2} & -\dfrac{\partial^2\varepsilon}{\partial\tilde{x}_2\partial\tilde{p}_2}\end{bmatrix}}_{M}\times\begin{bmatrix}\Delta\tilde{x}_1\\ \Delta\tilde{p}_1\\ \Delta\tilde{x}_2\\ \Delta\tilde{p}_2\end{bmatrix}. \tag{12}$$

Equations (9)–(12) are the basic relations we will use, after defining some further notation, to get the desired Jacobian determinant as a function of time.

A. Time-evolution matrix

The 4×4 matrix M in Eq. (12) is a function of the coordinates and momenta of our trajectory. Let us define the 4×4 evolution matrix $U(\tau)$:

$$\Delta Z(\tau)=\begin{bmatrix}\Delta\tilde{x}_1\\ \Delta\tilde{p}_1\\ \Delta\tilde{x}_2\\ \Delta\tilde{p}_2\end{bmatrix}\equiv U(\tau)\begin{bmatrix}\Delta\tilde{x}_{10}\\ \Delta\tilde{p}_{10}\\ \Delta\tilde{x}_{20}\\ \Delta\tilde{p}_{20}\end{bmatrix}=U(\tau)\Delta Z(0). \quad (13)$$

Substituting Eq. (13) into Eq. (12) we have

$$\frac{d}{d\tau}U(\tau)=MU(\tau). \quad (14)$$

Equation (14) is called the stability equation [9] of the classical trajectory. The initial condition for $U(\tau)$ is $U(0)=I$, where I is the unit matrix of dimension 4. $U(\tau)$ is independent of the choice of displacement $\Delta Z(0)$, once the initial phase-space point is chosen. We will use Eq. (14) in calculating $U(\tau)$, as described at the end of Sec. IV C.

From Eq. (13) we have

$$\begin{aligned}\Delta\tilde{x}_1&=u_{11}\Delta\tilde{x}_{10}+u_{12}\Delta\tilde{p}_{10}+u_{13}\Delta\tilde{x}_{20}+u_{14}\Delta\tilde{p}_{20}\\ \Delta\tilde{x}_2&=u_{31}\Delta\tilde{x}_{10}+u_{32}\Delta\tilde{p}_{10}+u_{33}\Delta\tilde{x}_{20}+u_{34}\Delta\tilde{p}_{20},\end{aligned} \quad (15)$$

where the u_{ij}'s are time-dependent elements of matrix $U(\tau)$. In a surface-of-section at $\tilde{x}_{10}=$constant [having chosen to use the variable $\tilde{x}_{20}$ in Eq. (7)], at a given time τ, from Eq. (15) we get the partial derivatives needed in Eq. (7) for calculating the Jacobian determinant:

$$\begin{aligned}\left(\frac{\partial\tilde{x}_1}{\partial\tilde{x}_{20}}\right)_{\tilde{x}_{10},\tau}&=u_{13}+u_{12}\left(\frac{\partial\tilde{p}_{10}}{\partial\tilde{x}_{20}}\right)_{\tilde{x}_{10}}+u_{14}\left(\frac{\partial\tilde{p}_{20}}{\partial\tilde{x}_{20}}\right)_{\tilde{x}_{10}},\\ \left(\frac{\partial\tilde{x}_2}{\partial\tilde{x}_{20}}\right)_{\tilde{x}_{10},\tau}&=u_{33}+u_{32}\left(\frac{\partial\tilde{p}_{10}}{\partial\tilde{x}_{20}}\right)_{\tilde{x}_{10}}+u_{34}\left(\frac{\partial\tilde{p}_{20}}{\partial\tilde{x}_{20}}\right)_{\tilde{x}_{10}}.\end{aligned} \quad (16)$$

Equation (16) is generally true for any energy-conserving Hamiltonian system. To use it, we need to calculate the partial derivatives at $\tau=0$, and then the evolution matrix elements u_{ij} at time τ.

B. Partial derivatives at $\tau=0$

From the Hamiltonian (2) of the coupled Morse oscillators we get

$$\tilde{p}_{10}=-\delta\tilde{p}_{20}\pm\sqrt{2\varepsilon-(1-\delta^2)\tilde{p}_{20}^2-2(1-e^{-\tilde{x}_{10}})^2-2(1-e^{-\tilde{x}_{20}})^2}. \quad (17)$$

The "+" in Eq. (17) corresponds to $\dot{\tilde{x}}_{10}>0$, and the "−" corresponds to $\dot{\tilde{x}}_{10}<0$. By differentiating both sides of Eq. (17) with respect to $\tilde{x}_{20}$, with ε constant and $\tilde{x}_{10}$ fixed, we obtain

$$\left(\frac{\partial\tilde{p}_{10}}{\partial\tilde{x}_{20}}\right)_{\tilde{x}_{10}}=-\delta\left(\frac{\partial\tilde{p}_{20}}{\partial\tilde{x}_{20}}\right)_{\tilde{x}_{10}}\mp\frac{(1-\delta^2)\tilde{p}_{20}\left(\dfrac{\partial\tilde{p}_{20}}{\partial\tilde{x}_{20}}\right)_{\tilde{x}_{10}}+2(1-e^{-\tilde{x}_{20}})e^{-\tilde{x}_{20}}}{\sqrt{2\varepsilon-(1-\delta^2)\tilde{p}_{20}^2-2(1-e^{-\tilde{x}_{10}})^2-2(1-e^{-\tilde{x}_{20}})^2}}, \quad (18)$$

where "−" corresponds to $\dot{\tilde{x}}_{10}>0$, and "+" corresponds to $\dot{\tilde{x}}_{10}<0$. To use Eq. (18) in Eq. (16), we need $(\partial\tilde{p}_{20}/\partial\tilde{x}_{20})_{\tilde{x}_{10}}$, which will be determined numerically from the classical torus, as described below in Sec. V.

C. Calculation of the time-evolution matrix

Next, using the Hamiltonian (2), the matrix M in Eq. (12) is

$$M=\begin{bmatrix}0 & 1 & 0 & \delta\\ 2(e^{-\tilde{x}_1}-2e^{-2\tilde{x}_1}) & 0 & 0 & 0\\ 0 & \delta & 0 & 1\\ 0 & 0 & 2(e^{-\tilde{x}_2}-2e^{-2\tilde{x}_2}) & 0\end{bmatrix}. \quad (19)$$

By substituting matrix M into Eq. (14) we get the set of differential equations

$$\frac{d}{d\tau}\begin{bmatrix}u_{12}\\ u_{22}\\ u_{32}\\ u_{42}\\ u_{13}\\ u_{23}\\ u_{33}\\ u_{43}\\ u_{14}\\ u_{24}\\ u_{34}\\ u_{44}\end{bmatrix}=\begin{bmatrix}u_{22}+\delta u_{42}\\ 2(e^{-\tilde{x}_1}-2e^{-2\tilde{x}_1})u_{12}\\ u_{42}+\delta u_{22}\\ 2(e^{-\tilde{x}_2}-2e^{-2\tilde{x}_2})u_{32}\\ u_{23}+\delta u_{43}\\ 2(e^{-\tilde{x}_1}-2e^{-2\tilde{x}_1})u_{13}\\ u_{43}+\delta u_{23}\\ 2(e^{-\tilde{x}_2}-2e^{-2\tilde{x}_2})u_{33}\\ u_{24}+\delta u_{44}\\ 2(e^{-\tilde{x}_1}-2e^{-2\tilde{x}_1})u_{14}\\ u_{44}+\delta u_{24}\\ 2(e^{-\tilde{x}_2}-2e^{-2\tilde{x}_2})u_{34}\end{bmatrix}, \quad (20)$$

with the initial condition $u_{ij}(0)=\delta_{ij}$ for $i=1, 2, 3, 4$ and $j=2,3,4$. Equations (20) are used to determine the τ-dependent matrix elements u_{12}, u_{13}, u_{14}, u_{32}, u_{33}, and u_{34} of $U(\tau)$ in Eq. (16). The differential equations for matrix elements u_{i1} for $i=1$, 2, 3, and 4 are decoupled from the other matrix elements in Eqs. (20), so they are irrelevant to our problem, and do not appear in Eq. (20). The time-dependent matrix $U(\tau)$ is not symmetric, as can be seen from Eq. (14) and Eq. (19).

To solve $U(\tau)$ numerically, we solve the equations of motion of the trajectory simultaneously with Eqs. (20). Except for one final step, treated in the next section, we now have all the ingredients needed for Eq. (16) and finally Eq. (7), the Jacobian determinant.

V. NUMERICAL CALCULATION OF SEMICLASSICAL WAVE FUNCTION FOR A QUANTIZING TORUS

To use Eqs. (16) and (18), we need $(\partial\tilde{p}_{20}/\partial\tilde{x}_{20})_{\tilde{x}_{10}}$. This has to be gotten numerically. To do this, it is useful to fit a small piece of the torus into a smooth curve expressed as an analytic function, and from this function calculate $(\partial\tilde{p}_{20}/\partial\tilde{x}_{20})_{\tilde{x}_{10}}$. The precision obtained has a strong effect on the accuracy of the Jacobian determinant.

In Ref. [1], we reported the result of a quantizing torus corresponding to the state (6, 3) of two kinetically coupled Morse oscillators with the following parameter values: $\delta=-0.014$, $D=44\,505.216\ \mathrm{cm}^{-1}$, $\omega_0=7.2916\times10^{14}\ \mathrm{s}^{-1}$, and $\beta=2.175\times10^{8}\ \mathrm{cm}^{-1}$.

The torus in the surface-of-section at $\tilde{x}_{10}=0$ around $\tilde{x}_{20}=0.323\,221\,125\,355\,621\,7\times10^{-4}$ was fit as

$$\tilde{p}_{20}=a_1+a_2\tilde{x}_{20}+a_3\tilde{x}_{20}^2, \tag{21}$$

where

$$a_1=0.962\,439\,573\,258\,279\,1,$$

$$a_2=-0.022\,471\,538\,043\,222\,85,$$

and

$$a_3=-1.015\,864\,044\,927\,796,$$

so

$$\left(\frac{\partial\tilde{p}_{20}}{\partial\tilde{x}_{20}}\right)_{\tilde{x}_{10}}=a_2+2a_3\tilde{x}_{20}=-0.022\,537\,207\,787\,184\,83. \tag{22}$$

We estimate that in actual fact, our calculated Jacobian determinant values were accurate to nine or ten significant figures.

The three-dimensional plot for the semiclassical wave function reported in Ref. [1] was obtained by calculating the wave function at 100×70 grid points. To generate the values at the grid lines along the $\tilde{x}_1$ axis direction, we used a surface-of-section at each $\tilde{x}_1$ value on the grid. The wave-function values on grid lines along the $\tilde{x}_2$ direction were obtained by an interpolation method. By using the data at the crossing points of these two sets of grid lines, the three-dimensional mesh plot was generated.

VI. CONCLUSION

In this Addendum to Ref. [1] we have presented details of our computation of a semiclassical wave function for coupled Morse oscillators, using the ''standard'' method of Maslov and Fedoriuk. This gave results in Ref. [1] equivalent to the new ''direct'' method developed there. Previously, Delos *et al.* [3] had shown that a numerical implementation of the standard method gives a good semiclassical wave function, using three trajectories, including two which in effect give the stability determinant. Our implementation of the standard method uses only a single trajectory, giving the stability with great numerical accuracy, at the cost of the cumbersome algebra presented here. Part of our motivation has been to achieve sufficient numerical accuracy to test the Maslov-Fedoriuk wave-function method on quantizing *cantori*, the chaotic remnants of EBK tori, shown by Davis [10] to be useful for semiclassical energies in the chaotic region. It may be that only the new ''direct'' method developed in [1] will have sufficient numerical stability to make this test. We hope to report on this in future work.

ACKNOWLEDGMENT

This work was supported by the U.S. Department of Energy Basic Energy Sciences program under Contract No. DE-FG03-98ER14848.

[1] S. Yang and M. E. Kellman, Phys. Rev. A **62**, 022105 (2000).
[2] V. P. Maslov and M. V. Fedoriuk, *Semiclassical Approximations in Quantum Mechanics* (D. Reidel, Dordrecht, Holland, 1981).
[3] S. K. Knudson, J. B. Delos, and D. W. Noid, J. Chem. Phys. **84**, 6886 (1986).
[4] A. Einstein, Verh. Dtsch. Phys. Ges. **19**, 82 (1917).
[5] J. B. Keller, Ann. Phys. (N.Y.) **4**, 180 (1958).
[6] R. T. Lawton and M. S. Child, Mol. Phys. **40**, 773 (1980).
[7] C. Jaffe and P. Brumer, J. Chem. Phys. **73**, 5646 (1980).
[8] E. L. Sibert, J. T. Hynes, and W. P. Reinhardt, J. Chem. Phys. **77**, 3583 (1982).
[9] J. M. Greene, in *Nonlinear Dynamics and the Beam-Beam Interaction*, edited by Melvin Month and John C. Herrea, AIP Conf. Proc. No. 57 (AIP, New York, 1979), pp. 257–271.
[10] M. J. Davis, J. Phys. Chem. **92**, 124 (1988); **107**, 106 (1997).