Semiclassical evaluation of inclusive transition probabilities

K. Möhring

Bereich Kern- und Strahlenphysik, Hahn-Meitner-Institut für Kernforschung Berlin GmbH, D-1000 Berlin-39, Federal Republic of Germany

U. Smilansky

Department of Nuclear Physics, The Weizman Institute of Science, Rehovot, Israel
(Received 7 October 1980; accepted 26 December 1980)

We develop a semiclassical description for reactions of complex particles based on Feynman's influence functional method. We study inclusive transition probabilities corresponding to a situation where only a set of collective variables is specified in the initial and the final states, for instance, inclusive angular distributions. We show that the inclusive probabilities can be expressed in terms of classical trajectories and derive proper equations of motion. We discuss to what extent interference phenomena appear, and present a uniform approximation for the description of focusing phenomena.

I. INTRODUCTION

The discussion of reactions between complex particles attracted recently an increasing degree of attention in various fields of physics. To list only a few examples, we can cite the investigation of deep inelastic collisions between heavy nuclei,[1] the detailed study of molecular collisions[2] and the scattering of ions from surfaces.[3] In all these areas, a rich body of experimental information is available, and it calls for the development of theoretical tools which could match the data in detail as well as in credibility.

A rigorous treatment of the complicated scattering problem is beyond present day theoretical and computational scope. Instead various approximate methods were developed. A feature common to most of these methods is the separation of the relevant degrees of freedom into two classes. The first includes the "collective" (macroscopic) degrees of freedom. Often the experimental observables are functions of these variables. Sometimes they are characterized as the "slow" variables and they appear *explicitly* as the variables in any theoretical study. The distance between the two reactants in a collision is such a degree of freedom. The second class of degrees of freedom is the "intrinsic" (microscopic) set (sometimes they are referred to as the "bath"). Their coupling to the collective variables is responsible for dissipation and relaxation phenomena. One follows their development only to the extent and detail needed for calculating their effect on the motion of the collective variables.

There exists no rigorous algorithm to extract the relevant collective variables for any given problem. In practical applications the distinction is made on the basis of physical intuition and convenience. We shall not investigate this problem, but rather assume that the Hamiltonian function which describes the complete system is already written down in terms of "collective" and "bath" degrees of freedom. We shall consistently denote collective variables by upper case letters, whereas for the bath variables we shall use lower case symbols.

In the present paper we shall address ourselves to the calculation of inclusive transition probabilities for the collective subsystem (macrosystem). That is we shall calculate the probability that in a given time interval T, the macrosystem develops from its initial to the final state, while the microsystem propagates from its initial state to any final state. The problem of calculating the inclusive transition probability is the simplest nontrivial task in the theoretical investigation of complex reactions. Our approach will be based on the observation that for many purposes the description of the collective degrees of freedom in terms of the semiclassical approximation is sufficiently accurate. We shall show that the study of the inclusive probability leads to a natural definition of the "mean" classical trajectory. We shall also show that under some conditions we can get useful information concerning the distribution of observables in the intrinsic system. Feynman's influence functional method[4] will be used for the semiclassical treatment of inclusive transition probabilities. The influence functional will be introduced in Sec. II. The semiclassical approximation will be derived by applying the saddle-point method for the relevant path integrals. The saddle-point condition results in the equations of motion for the "mean" ("inclusive") trajectory which will be presented in Sec. III. The calculation of the inclusive probability will be performed and presented in Sec. IV. We shall also investigate to what extent quantal interference effects survive after the integration over all final intrinsic states is performed. This will be done together with the discussion of a "uniform" semiclassical expression which is needed in the presence of classical focussing. Such focusing is seen for instance as rainbow scattering in the inclusive angular distribution of heavy ions[1] as well as in the scattering of ions from molecules.[2]

The equations of motion derived in the present formalism are related to the semiclassical approximation developed by Pechukas[5] and they can also be discussed in the context of the self-consistent mean field approximation.[6] A comparison between our results and those of Refs. 5 and 6 will be given in Sec. V. It will enable us

 0021-9606/81/084509-10$01.00

to assess the range of validity of some of our approximations.

The work reported here is a generalization of our previous study[7] in which the same problem was discussed but special models where assumed for the bath and its coupling to the collective variables. That is, we assumed the bath to be either weakly coupled (linear response) or to consist of harmonic oscillators linearly coupled to the collective modes. Under these assumptions one gets explicit expressions for the influence functional in terms of the collective variables. The main point of the present report is to show that most of our previous results can be generalized and are valid under the most general conditions.

II. THE PATH INTEGRAL

We start by presenting a quantum-mechanical expression for the inclusive transition probability, which will offer the most convenient ground for the semiclassical approximation. We denote the collective coordinates by $\mathbf{R}$ and their canonically conjugate momenta by $\mathbf{P}$. The microvariables will be denoted by $\mathbf{r}$ and p, respectively. Let $H(\mathbf{R}, \mathbf{P}, \mathbf{r}, \mathrm{p})$ be the Hamiltonian function of the complete system.

For the sake of simplifying the notation we shall assume that the macrosystem contains just one degree of freedom. All the results can be generalized to the multidimensional case in a straightforward manner.

The inclusive probability we are going to consider, is the probability that in a given time interval T the collective motion develops from R_i to R_f while the microsystem propagates from its ground state $|0\rangle$ to any final state $|n\rangle$. Thus, the transition probability is summed over all the final states $|n\rangle$ of the microsystem

$$P_{\mathrm{incl}}(R_i;R_f;T)=\sum_n P(R_i, 0;R_f, n;T) . \qquad (2.1)$$

For the semiclassical approximation the most convenient formulation of quantum mechanics is the language of Feynman's path integrals.[4] Originally Feynman used a Lagrangian description when he introduced the path integral concept, and the paths were defined in coordinate space. This approach was taken also in Ref. 7. In the present paper we shall use the Hamiltonian formulation[8] because it covers a more general class of physical problems. Here we have to integrate over paths in phase space. The quantum-mechanical propagator reads (with $\hbar=1$)

$$K(R_i;\mathbf{r}_i, R_f, \mathbf{r}_f;T)$$
$$=\int D[R, P]D[\mathbf{r}, \mathrm{p}]\exp\left\{i\int_0^T dt(P\dot{R}+\mathrm{p}\dot{\mathbf{r}}-H)\right\} . \qquad (2.2)$$

The path integral goes over all paths $R(t)$, $P(t)$, $\mathbf{r}(t)$, $\mathbf{p}(t)$, which satisfy the boundary conditions

$$R(0)=R_i , \quad R(T)=R_f , \quad \mathbf{r}(0)=\mathbf{r}_i , \quad \mathbf{r}(T)=\mathbf{r}_f . \qquad (2.3)$$

Taking proper matrix elements $\langle n|K|0\rangle$ with respect to the initial and final states of the microsystem, squaring and summing over all the final states $|n\rangle$, we may write the inclusive probability (2.1) as

$$P_{\mathrm{incl}}(R_i;R_f;T)=\int D[R, P]$$
$$\times\ D[\tilde{R}, \tilde{P}]\exp\left[i\int_0^T dt(P\dot{R}-\tilde{P}\dot{\tilde{R}})\right]F[R, P;\tilde{R}, \tilde{P}] . \qquad (2.4)$$

The right-hand side is a double path integral over the product space of paths $[R,(t), P(t)]$ and $[\tilde{R}(t), \tilde{P}(t)]$ for the macrosystem. Both paths have to satisfy the boundary conditions (2.3). All the dependence upon the microsystem is comprised in the "influence functional":

$$F[R, P;\tilde{R}, \tilde{P}]=\sum_n \langle 0|K^{+}_{[\tilde{R}, \tilde{P}]}|n\rangle\langle n|K_{[R, P]}|0\rangle . \qquad (2.5)$$

The propagator

$$K_{[R,P]}=\int D[\mathbf{r}, \mathrm{p}]\exp\left\{i\int_0^T dt(\mathrm{p}\dot{\mathbf{r}}-H(R(t), P(t), \mathbf{r}, \mathrm{p})\right\} \qquad (2.6)$$

drives the microsystem which is coupled to the macrosystem while the latter follows the prescribed path $[R(t), P(t)]$. $K_{[R,P]}$ is a functional of that path. The influence functional can be written in a more condense way. We consider the Schrödinger equation

$$i\frac{\partial}{\partial t}\ |\varphi_{[R,P]}(t)\rangle=H[R(t), P(t)]|\varphi_{[R,P]}(t)\rangle , \qquad (2.7)$$

with the initial condition

$$|\varphi_{[R,P]}(0)\rangle=|0\rangle . \qquad (2.8)$$

Here $H(R, P)$ is an operator in the Hilbert space of the microsystem which depends parametrically upon the given macropath $[R(t), P(t)]$. Therefore, H is explicitly time dependent. The influence functional (2.5) can be easily identified as

$$F[R, P;\tilde{R}, \tilde{P}]=\langle\varphi_{[\tilde{R},\tilde{P}]}(T)|\varphi_{[R,P]}(T)\rangle . \qquad (2.9)$$

We introduce the abbreviated notation

$$\varphi_0(t)=\varphi_{[R,P]}(t) , \quad \tilde{\varphi}_0(t)=\varphi_{[\tilde{R},\tilde{P}]}(t) , \qquad (2.10)$$

where the subscripts refer to the initial condition (2.8), and write the inclusive probability (2.4) as

$$P_{\mathrm{incl}}(R_i;R_f;T)$$
$$=\int D[R, P]\int D[\tilde{R}, \tilde{P}]\exp\{iS_{\mathrm{eff}}[R, P;\tilde{R}, \tilde{P}]\} , \qquad (2.11)$$

$$S_{\mathrm{eff}}[R, P; \tilde{R}, \tilde{P}]=\int_0^T dt\,(P\dot{R}-\tilde{P}\dot{\tilde{R}})-i\ln\langle\tilde{\varphi}_0(T)|\varphi_0(T)\rangle . \qquad (2.12)$$

III. THE CLASSICAL EQUATIONS OF MOTION

We proceed by evaluating the double path integral (2.11) in the stationary phase approximation. That is, we assume that the main contribution to the integral comes from the neighborhood of those paths for which the effective action (2.12) has a vanishing first variation. The latter condition will define classical equations of motion for the macropaths (R, P) and $(\tilde{R}, \tilde{P})$. The approximation is therefore equivalent to a semiclassical description of the macrosystem whereas the microsystem is still treated quantum mechanically.

In order to deduce the equations of motion we study the first variation of the action (2.12) with respect to both the paths (R, P) and $(\tilde{R}, \tilde{P})$,

$$\delta S_{eff} = \int_0^T dt(\delta P\dot{R} - \delta R\dot{P} - \delta\tilde{P}\dot{\tilde{R}} + \delta\tilde{R}\dot{\tilde{P}}) - \frac{i}{\langle\tilde{\varphi}_0(T)|\varphi_0(T)\rangle}[\langle\tilde{\varphi}_0(T)|\delta\varphi_0(T)\rangle + \langle\delta\tilde{\varphi}_0(T)|\varphi_0(T)\rangle]. \tag{3.1}$$

The solution $|\varphi_0(t)\rangle$ of Eqs. (2.7) and (2.8) depends upon the path (R, P) via the Hamiltonian. Operating with the variation of Eq. (2.7) we find that $|\delta\varphi_0(t)\rangle$ satisfies

$$i\frac{\partial}{\partial t}|\delta\varphi_0(t)\rangle = H[R, P]|\delta\varphi_0(t)\rangle + \left(\frac{\partial H}{\partial R}\delta R + \frac{\partial H}{\partial P}\delta P\right)|\varphi_0(t)\rangle, \tag{3.2}$$

with the initial condition

$$|\delta\varphi_0(0)\rangle = 0. \tag{3.3}$$

We define a set of solutions $|\varphi_n(t)\rangle$ to Eq. (2.7) by imposing the initial conditions

$$|\varphi_n(0)\rangle = |n\rangle. \tag{3.4}$$

It is easily shown that at every time t the $|\varphi_n(t)\rangle$ are orthonormal and complete,

$$\langle\varphi_n(t)|\varphi_m(t)\rangle = \delta_{nm}, \tag{3.5}$$

$$\sum_n |\varphi_n(t)\rangle\langle\varphi_n(t)| = 1. \tag{3.6}$$

Expanding $|\delta\varphi_0\rangle$ in this basis we find

$$|\delta\varphi_0(t)\rangle = \frac{1}{i}\sum_n |\varphi_n(t)\rangle \int_0^t ds\langle\varphi_n(s)|\frac{\partial H}{\partial R}\delta R + \frac{\partial H}{\partial P}\delta P|\varphi_0(s)\rangle. \tag{3.7}$$

This expression together with the analogous one for $|\delta\tilde{\varphi}_0\rangle$ is substituted into Eq. (3.1). Isolating the factors which multiply the different variations on the right-hand side we find the equation for the stationary paths,

$$\begin{aligned}\dot{R} &= \sum_n \frac{\langle\tilde{\varphi}_0(T)|\varphi_n(T)\rangle}{\langle\tilde{\varphi}_0(T)|\varphi_0(T)\rangle}\langle\varphi_n(t)|\frac{\partial H}{\partial P}|\varphi_0(t)\rangle, \\ \dot{P} &= -\sum_n \frac{\langle\tilde{\varphi}_0(T)|\varphi_n(T)\rangle}{\langle\tilde{\varphi}_0(T)|\varphi_0(T)\rangle}\langle\varphi_n(t)|\frac{\partial H}{\partial R}|\varphi_0(t)\rangle.\end{aligned} \tag{3.8}$$

Two similar equations hold for the path $(\tilde{R}, \tilde{P})$. The right-hand sides of these equations are complex valued so that Eqs. (3.8) represent in fact four equations. The imaginary parts of Eqs. (3.8) vanish when

$$\frac{\langle\tilde{\varphi}_0(T)|\varphi_n(T)\rangle}{\langle\tilde{\varphi}_0(T)|\varphi_0(T)\rangle} = \delta_{n0}. \tag{3.9}$$

Then *both* paths (R, P) and $(\tilde{R}, \tilde{P})$ have to satisfy

$$\begin{aligned}\dot{R}(t) &= \langle\varphi_0(t)|\frac{\partial H}{\partial P}|\varphi_0(t)\rangle, \\ \dot{P}(t) &= -\langle\varphi_0(t)|\frac{\partial H}{\partial R}|\varphi_0(t)\rangle,\end{aligned} \tag{3.10}$$

with

$$R(0) = \tilde{R}(0) = R_i, \quad R(T) = \tilde{R}(T) = R_f. \tag{3.11}$$

The only coupling between the two paths is the condition (3.9) which is equivalent to

$$|\tilde{\varphi}_0(T)\rangle = e^{i\alpha}|\varphi_0(T)\rangle, \tag{3.12}$$

where α is a real phase. A stationary point of the double path integral (2.11) is defined by a pair of trajectories which simultaneously solve the "classical" equations of motion (3.10) and (3.11) and the Schrödinger Eqs. (2.7) and (2.8) subject to the additional condition (3.12).

Equations (3.10) are Hamilton's equations of motion averaged with the microsystem wave function as obtained from the Schrödinger equation (2.7). But because the wave function depends upon the path, Eqs. (3.10) cannot be deduced from a classical (average) Hamiltonian function. They constitute a nonconservative, dissipative problem.

The energy loss along a solution (R, P) of Eqs. (3.10) and (2.7) is easily calculated. Along the trajectory

$$\frac{d}{dt}\langle\varphi_0(t)|H[R(t), P(t)]|\varphi_0(t)\rangle = 0. \tag{3.13}$$

Assuming the macro and microsystem to be decoupled at both ends of the trajectory, we find that the classical path (R, P) loses the energy

$$E(T) - E(0) = -\{\langle\varphi_0(T)|h|\varphi_0(T) - \langle 0|h|0\rangle\}. \tag{3.14}$$

Here h is the Hamiltonian of the isolated microsystem.

The equations of motion (3.10) define the paths which determine the inclusive probability via the stationary phase approximation. Therefore these trajectories can be considered as the mean trajectories of the macrosystem in an inclusive experiment. Correspondingly the equations of motion do not contain any fluctuating force. We will discuss in Sec. V to what extent we may use the mean trajectories to extract information on distributions in the final state of the system.

The formalism discussed above can be easily generalized to situations where the intrinsic system is initially defined as an incoherent state with a given probability distribution (= density matrix). Thus, the expectation values which appear on the right-hand side of Eq. (3.8) should now be taken with the help of the density matrix $\rho(t)$. The later develops by the time-dependent von Neumann equation which generalizes Eq. (2.7).

In Ref. 7, we discussed a special class of microsystems. We considered three situations: A harmonic microsystem with linear coupling to the macrosystem, and microsystems which are coupled in such a way that either first-order perturbation theory or the adiabatic limit hold. These problems have in common that the Schrödinger Eq. (2.7) can be solved analytically and the right-hand side of Eqs. (3.10) can be spelt out explicitly in terms of the trajectory, leading to formally identical expressions in all three cases.

IV. THE INCLUSIVE PROBABILITY

Considering the various possible stationary points to the double path integral (2.11) we may distinguish two basically different cases. In the first case the two paths constituting the stationary point are identical, in the second they are different.

Let us begin with the first case. When the two paths (R, P) and $(\tilde{R}, \tilde{P})$ are identical, the condition (3.12) is satisfied identically. In other words, every solution of the boundary value problem (3.10) and (3.11) solved simultaneously with the Schrödinger Eqs. (3.7) and (3.8) represents a stationary point of the path integral (2.11).

In order to calculate the contribution of such a stationary point to the integral we proceed with the stationary phase approximation. We calculate the second variation of the effective action (2.12) and evaluate the corresponding double Gaussian path integral around the stationary point

$$P_{(R,P)} = \int D[\delta R, \delta P] \int D[\delta \tilde{R}, \delta \tilde{P}] \exp[(i/2)\delta^2 S_{\text{eff}}] . \tag{4.1}$$

$\delta^2 S_{\text{eff}}$ is a quadratic form in the variations δ and (R, P) is the trajectory representing the stationary point. The evaluation of this Gaussian integral is the content of Appendix A. We find the classical result

$$P_{(R,P)} = \frac{1}{2\pi} \left| \frac{\partial R(T)}{\partial P(0)} \right|^{-1} . \tag{4.2}$$

The transition probability along the trajectory (R, P) is given by the inverse of the van Vleck "determinant" of the derivative of the final "coordinate" $R(T)$ with respect to the initial "momentum" $P(0)$. This supports the interpretation of (R, P) as a mean trajectory. It is the classical phase space factor along this trajectory which determines the corresponding inclusive probability.

Operationally, we proceed like in the conventional semiclassical approach. Starting from R_i and varying the initial conjugate momentum $P(0)$ through the range of possible values we create the "deflection function" $R(T)$ as a function of $P(0)$. From that we determine those values of $P(0)$ which lead to the desired R_f. The derivative of the "deflection function" determines the probability (4.2). This derivative is the R component of the stability field which describes the variation of the trajectory with the initial momentum $P(0)$. It may also be obtained by solving the corresponding stability equation given in Appendix A.

Compared to the conventional semiclassics we still miss interference terms as they may appear when to the given R_f there contribute more than one classical trajectory. This interference is given by the second class of stationary points mentioned at the beginning of this section.

Let us assume that there are two trajectories leading to R_f, i.e., two solutions of Eqs. (3.10) and (3.11) and (2.7) and (2.8). Such a pair of paths may constitute a stationary point of the double path integral (2.11) which we would clearly interpret as due to interference between the two trajectories. However, the two have to satisfy the additional condition (3.12) that at $t = T$ the two wave functions of the microsystem as propagated along the two different trajectories must be physically identical. Considering any nontrivial microsystem we realize that there is practically no chance to satisfy such a requirement. In other words, the corresponding stationary points are shifted into the complex plane and represent only exponentially small contributions to the double path integral.

We therefore draw the conclusion that for the inclusive probability contributions due to interference can well be neglected and we stay with the "classical" contributions (4.2).

There is, however, still one remaining manifestation of quantum mechanics. $R(T)$ as a function of $P(0)$ may exhibit an extremum. In the neighborhood of such an extremum the right-hand side of Eq. (4.2) gets very large. We meet a classical catastrophe or focus where at least two classical trajectories coalesce. The treatment which resulted in Eq. (4.2) and which was based on the assumption that the stationary points are well separated, breaks down. We have to go beyond the "primitive" stationary phase approximation by introducing the proper uniformization. [8]

We restrict ourselves to the simplest case and consider two coalescing stationary points. In a conventional semiclassical treatment of transition amplitudes such a case would call for an Airy-type uniformization. The present problem is slightly more complicated because we deal with a double path integral which has two real-valued stationary points and two complex ones as discussed above.

The way how to derive the proper uniformization is described in Appendix B. The resulting expression for the inclusive probability reads

$$P_{\text{incl}} = (P_{(R_1,P_1)} + P_{(R_2,P_2)}) |\xi|^{-1/2} I(\xi, \eta) , \tag{4.3}$$

with

$$I(\xi, \eta) = \frac{1}{\sqrt{\pi}} \int_0^\infty \frac{dx}{\sqrt{x}} e^{-\eta x^2} \cos\left(\xi x - \frac{x^3}{12} - \frac{\pi}{4}\right) . \tag{4.4}$$

Here (R_1, P_1) and (R_2, P_2) are the two classical trajectories representing the two contributing stationary points. The parameters ξ and η are defined in terms of the "mixed" effective action $S_{\text{eff}}(R_1, P_1; R_2, P_2)$ as given by Eq. (2.12). They are

$$\xi = [\tfrac{3}{8}[S_{\text{eff}}(R_2, P_2; R_1, P_1) - S_{\text{eff}}(R_1, P_1; R_2, P_2)]]^{2/3} \tag{4.5}$$

and

$$\eta = \frac{1}{8i} \xi^{-1}[S_{\text{eff}}(R_2, P_2; R_1, P_1) + S_{\text{eff}}(R_1, P_1; R_2, P_2)] . \tag{4.6}$$

We note that at the focus both ξ and η go to zero. The integral (4.4) stays finite and the factor $\xi^{-1/2}$ in (4.3) cancels the classical divergence of the $P_{(R_i,P_i)}$. The probability (4.3) remains finite at the focus. In deriving Eqs. (4.3) and (4.4) the complex stationary points were taken into account only in an approximate fashion, consistent with the fact that the corresponding interference terms do not really contribute to the inclusive probability. Still, inspecting the structure of the integral I as given in Fig. 1, we find some reminiscence of an interference pattern. The parameter η differs from zero only when the overlap $|\langle \tilde{\varphi}_0(T) | \varphi_0(T) \rangle|$ differs from 1. Therefore, η measures to what extent the two classical trajector-

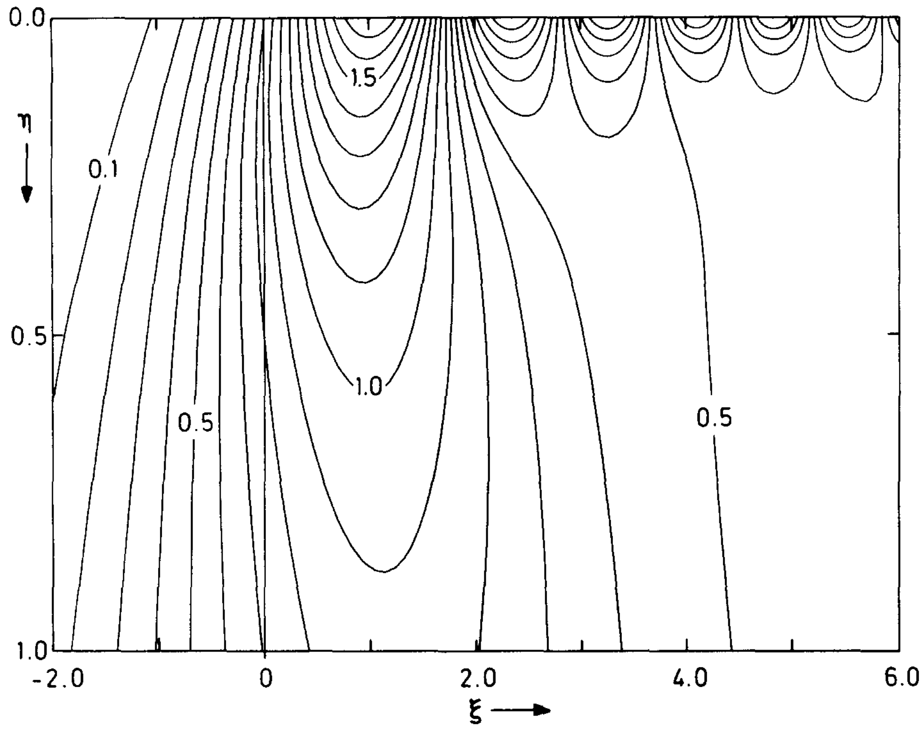

FIG. 1. A contour plot of the uniformizing integral $I(\xi, \eta)$ defined by Eq. (4.4).

ies violate the interference condition (3.12). Correspondingly $I(\xi, \eta)$ shows some oscillatory behavior on the bright side of the focus ($\xi > 0$) when η is sufficiently small.

Calculations at the shadow side of the focus (classically forbidden transitions) would require complex-valued trajectories. Instead, we propose a crude but simpler approximation based on a quadratic expansion around the focus. The resulting expression for the classical probabilities together with the parameters ξ and η are also given in Appendix B.

For $\xi \to \infty$ (well separated trajectories) the expression (4.3) again reduces to the classical result, namely, we get the sum of the two classical probabilities.

V. DISCUSSION

In the preceding sections we derived a semiclassical approximation for the inclusive transition probability. It is obtained in terms of the "inclusive" classical trajectories for the macrosystem. We established classical equations of motion which are to be solved simultaneously with a Schrödinger equation for the microsystem. The form of these equations appears to be quite natural. As stated by several authors (cf., e.g., Refs. 9–11), they can, once the macrosystem is assumed to behave classically, be derived by just applying Ehrenfest's theorem. The classical motion of the macrosystem is governed by the coupling to the microsystem averaged with the quantum-mechanical wave function of the microsystem, as the latter is not observed in the inclusive probability.

The analysis of the underlying path integral allowed the discussion of interference and, in particular, focusing effects. We find that, apart from focusing, the manifestation of interferences between different inclusive trajectories is quite improbable. For a proper uniformization of the semiclassical inclusive probability next to a focus the formalism provides all the necessities. For the simplest case of two coalescing trajectories we present the uniformization explicitly.

We may conclude with the question to what extent the proposed semiclassical description of the collision process may provide information beyond the inclusive probabilities. Strictly speaking, the wave function of the microsystem is only an auxiliary quantity for the purpose of calculating the classical inclusive trajectory. As discussed by Willis and Picard[6] the Schrödinger equation (2.7) represents a mean field approximation. Using it to describe the microsystem is justified only when the correlations between the two subsystems leave the density matrix of the entire system factorized into a macro and a microdensity matrix. (The correlations required for the calculation of the inclusive probability are taken into account correctly.) We did not fully recognize this point in our previous publication[7] when discussing the distribution of the transferred energy. Some of our statements there should be modified.

Accepting the mean field approximation we can easily calculate the mean and the width of the final energy distribution in the microsystem. The result is

$$\langle e \rangle = \langle \varphi_0(T) | h | \varphi_0(T) \rangle \tag{5.1}$$

and

$$\sigma(e) = \{ \langle \varphi_0(T) | h^2 | \varphi_0(T) \rangle - \langle e \rangle^2 \}^{1/2} . \tag{5.2}$$

This should provide a fair description as long as the distribution is narrow. The mean energy gained by the microsystem appears to be equal to the energy (3.14) lost from the macrosystem. Similarly the amount of angular momentum lost from the macrosystem along the trajectory equals to the gain in intrinsic spin by the microsystem. These results reflect the consistent treatment of both the macro and the microsystem in the mean field approximation.

A proper description of the final state of the microsystem within the semiclassical approximation was provided by the work of Pechukas.[5] He proposed a semiclassical approximation for the transition probability $P(R_i, 0; R_f, n; T)$ to a given final state n of the microsystem (cf. Sec. II). His result is

$$P(R_i, 0; R_f, n; T) = |\langle n|\varphi_0^{(n)}(T)\rangle|^2 \frac{1}{2\pi}\left|\frac{\partial R_n(T)}{\partial P_n(0)}\right|^{-1} . \qquad (5.3)$$

Here, (R_n, P_n) is a classical trajectory which satisfies the equations of motion

$$\dot{R}_n(t) = \mathrm{Re}\left\{\sum_m \frac{\langle n|\varphi_m^{(n)}(T)\rangle}{\langle n|\varphi_0^{(n)}(T)\rangle}\langle\varphi_m^{(n)}(t)|\ \frac{\partial H}{\partial P}\ |\varphi_0^{(n)}(t)\rangle\right\} ,$$
$$\dot{P}_n(t) = -\mathrm{Re}\left\{\sum_m \frac{\langle n|\varphi_m^{(n)}(T)\rangle}{\langle n|\varphi_0^{(n)}(T)\rangle}\langle\varphi_m^{(n)}(t)|\ \frac{\partial H}{\partial R}\ |\varphi_0^{(n)}(t)\rangle\right\} , \qquad (5.4)$$

with the boundary condition (2.3). The $\varphi_m^{(n)}(t)$ solve the Schrödinger Eq. (2.7) along the path (R_n, P_n) with the initial condition

$$|\varphi_m^{(n)}(0)\rangle = |m\rangle . \qquad (5.5)$$

Equations (5.4) demand the *a priori* knowledge of the wave functions $\varphi_m^{(n)}(T)$ at the end of the trajectory. As the equations are coupled to the corresponding Schrödinger equation, they can be solved only iteratively. This complication reflects the fact that we are interested in a particular final state of the microsystem. Similarly, when together with the macrosystem also the microsystem can be treated semiclassically,[11,12] the trajectories are defined via a highly dimensional boundary value problem. Only for the inclusive probability where no final information about the microsystem is required, the classical problem reduces to a pure initial value problem as far as the microsystem is concerned.

Expression (5.3) offers a more transparent interpretation of the inclusive trajectory as a mean trajectory. The transition probability to a given final state n is given via a specific classical trajectory (R_n, P_n) which depends upon this state. The probability is given by the the corresponding phase space factor multiplied by the "excitation probability" $|\langle n|\varphi_0^{(n)}(T)\rangle|^2$. Summing Eq. (5.3) over all n and comparing to Eq. (4.2) we find

$$\left|\frac{\partial R(T)}{\partial P(0)}\right|^{-1} = \sum_n |\langle n|\varphi_0^{(n)}(T)\rangle|^2\left|\frac{\partial R_n(T)}{\partial P_n(0)}\right|^{-1} . \qquad (5.6)$$

Thus, the inclusive trajectory (R, P) is a mean trajectory in the sense that its phase space factor (van Vleck determinant) is the mean of phase space factors calculated along the classical trajectories to the individual final states $|n\rangle$ weighted by the corresponding excitation probabilities.

In many cases of practical interest, the trajectories (R_n, P_n) corresponding to final states which exhaust most of the excitation probabilitiy, are rather similar. Then the inclusive trajectory (R, P) can be taken to approximate them, so that

$$P(R_i, 0; R_f, n; T) \cong |\langle n|\varphi_0(T)\rangle|^2 \frac{1}{2\pi}\left|\frac{\partial R(T)}{\partial P(0)}\right|^{-1} , \qquad (5.7)$$

where all the quantities are calculated along the inclusive trajectory. This is again the mean field approximation. Its practical advantage is apparent, especially if one compares the equations of motion (3.10) and (5.4). Summed over all n, Eq. (5.7) is again semiclassically exact.

An alternative improvement of the mean field approximation can be achieved along the lines of Ref. 6. Some progress in this direction will be reported in Ref. 13. It leads to a Fokker–Planck like equation for the classical motion of the macrosystem whereas the dynamics of the microsystem which determines the transport coefficients, is governed by the Hamiltonian averaged over the classical phase space distribution of the macrosystem. It seems, however, that by such an approach one is restricted to the purely classical description of the macro degrees of freedom excluding a proper description of focusing.

ACKNOWLEDGMENT

We would like to express our gratitude to Dr. D. H. E. Gross and Dr. S. Mukamel for enlightening discussions and comments. We are also indebted to the Department of Physics of the Weizman Institute and the Hahn–Meitner-Institute for supporting our collaboration.

APPENDIX A

In this Appendix we evaluate the Gaussian double path integral (4.1)

$$P_{(R,P)} = \int D[\delta R, \delta P]\int D[\delta\tilde{R}, \delta\tilde{P}]\exp\left(\frac{i}{2}\,\delta^2 S_{\mathrm{eff}}\right) \qquad (\mathrm{A}1)$$

by techniques which were essentially developed in Refs. 7 and 8.

The result is given by Eq. (4.2). The right-hand side contains the van Vleck determinant $\partial R(T)/\partial P(0)$ which is related to the classical stability equations. They result from derivating the classical equation of motion (3.9) with respect to the initial momentum $P(0)$. In matrix notation

$$\left(\Gamma\,\frac{d}{dt} - \Theta\right)\xi = 0, \quad \xi(0) = \begin{pmatrix}0\\1\end{pmatrix} . \qquad (\mathrm{A}2)$$

Γ and Θ are 2×2 matrices,

$$\Gamma = \begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix} \qquad (\mathrm{A}3)$$

and

$$\Theta = \begin{pmatrix}\frac{\partial}{\partial R}\langle\varphi_0|\ \frac{\partial H}{\partial R}\ |\varphi_0\rangle & \frac{\partial}{\partial P}\langle\varphi_0|\ \frac{\partial H}{\partial R}\ |\varphi_0\rangle\\ \frac{\partial}{\partial R}\langle\varphi_0|\ \frac{\partial H}{\partial P}\ |\varphi_0\rangle & \frac{\partial}{\partial P}\langle\varphi_0|\ \frac{\partial H}{\partial P}\ |\varphi_0\rangle\end{pmatrix} . \qquad (\mathrm{A}4)$$

$\xi = \binom{x}{y}$ is a two-dimensional vector and obviously $x(T) = \partial R(T)/\partial P(0)$.

It should be noticed that Θ is an integral operator (of Volterra-type) as is easily seen with the help of Eq. (3.7).

In order to calculate the integral (A1) we first write down the second variation of the effective action explicitly. After some straightforward algebra, again using Eq. (3.7) and the equivalent for $|\delta\varphi_n\rangle$, we obtain *at the stationary point*,

$$\delta^2 S_{\rm eff} = \int_0^T dt\, \delta Q\left(\Gamma \frac{d}{dt} - \Theta\right)\delta Q - \int_0^T dt\, \delta\tilde{Q}\left(\Gamma\frac{d}{dt} - \Theta\right)\delta\tilde{Q} - \int_0^T dt \int_0^T ds \left\{\delta Q(t)\Phi(t,s)\delta Q(s) - 2\delta Q(t)\Phi(t,s)\delta\tilde{Q}(s) + \delta\tilde{Q}(t)\Phi(t,s)\delta\tilde{Q}(s)\right\} . \quad \text{(A5)}$$

We isolated the stability operator $\Gamma(d/dt)-\Theta$ of Eq. (A2). δQ and $\delta\tilde{Q}$ are the path variations

$$\delta Q = \begin{pmatrix}\delta R\\ \delta P\end{pmatrix}, \quad \delta\tilde{Q} = \begin{pmatrix}\delta\tilde{R}\\ \delta\tilde{P}\end{pmatrix} , \quad \text{(A6)}$$

and Φ is the matrix

$$\Phi(t,s) = \begin{pmatrix}\Phi_{RR}, \Phi_{RP}\\ \Phi_{PR}, \Phi_{PP}\end{pmatrix} , \quad \text{(A7)}$$

with

$$\Phi_{xy} = \frac{1}{i}\sum_n \langle\varphi_0(t)|\,\frac{\partial H}{\partial x}\,|\varphi_n(t)\rangle\langle\varphi_n(s)|\,\frac{\partial H}{\partial y}\,|\varphi_0(s)\rangle . \quad \text{(A8)}$$

Next, we introduce a path expansion scheme as discussed in Ref. 8. As a basis we use the eigenfunctions of the differential operator $\Gamma(d/dt)$

$$\Gamma\frac{d}{dt}\chi^{(\gamma)}(t) = \varphi_\gamma \chi^{(\gamma)}(t) , \quad \text{(A9)}$$

$$\chi^{(\gamma)}(t) = \begin{pmatrix}u^{(\gamma)}(t)\\ v^{(\gamma)}(t)\end{pmatrix} , \quad \text{(A10)}$$

for the boundary conditions

$$u^{(\gamma)}(0) = u^{(\gamma)}(T) = 0 . \quad \text{(A11)}$$

There is one vanishing eigenvalue,

$$\varphi_0 = 0 , \quad \text{(A12)}$$

the corresponding eigenfunction reads

$$\chi^{(0)}(t) = \frac{1}{\sqrt{T}}\begin{pmatrix}0\\ 1\end{pmatrix} . \quad \text{(A13)}$$

$\Gamma(d/dt)$ being Hermitian in the considered path-space, the path variation can be represented as

$$\delta Q(t) = \sum_{\gamma=0}^{\infty} a_\gamma \chi^{(\gamma)}(t) , \qquad \delta\tilde{Q}(t) = \sum_{\gamma=0}^{\infty}\tilde{a}_\gamma\chi^{(\gamma)}(t) , \quad \text{(A14)}$$

and the path integral can be rewritten as an integral over all the expansion coefficients. Truncating the expansion (A14) at $\gamma = N$ we get the Nth approximant to the integral

$$P^{(N)}_{(R,P)} = \int_{-\infty}^{+\infty}\prod_{\gamma=0}^{N} da_\gamma d\tilde{a}_\gamma J_N \exp\left[\frac{i}{2}\,\delta^2 S_{\rm eff}(\{a_\gamma,\tilde{a}_\gamma\})\right] . \quad \text{(A15)}$$

The Jacobian J_N is deduced in Ref. 8. It is (for the double path integral)

$$J_N = \frac{1}{(2\pi)^2}\prod_{\gamma=1}^{N}\frac{\varphi_\gamma}{2\pi i} . \quad \text{(A16)}$$

Performing the integral we find

$$P^{(N)}_{(R,P)} = \frac{1}{2\pi T}\prod_{\gamma=1}^{N}\varphi_\gamma \Omega^{-1/2} , \quad \text{(A17)}$$

where Ω is the determinant of essentially all the $(2N+2)\times(2N+2)$ 2nd derivatives of $\delta^2 S_{\rm eff}$ with respect to the coefficients a_γ and $\tilde{a}_\gamma$. Explicitly we obtain at the stationary point

$$\Omega = -\det\begin{pmatrix}A & B\\ -B^T & C\end{pmatrix} , \quad \text{(A18)}$$

with the $(N+1)\times(N+1)$ matrices

$$A_{\gamma\gamma'} = \int_0^T dt\,\chi^{(\gamma')}\left(\Gamma\frac{d}{dt}-\Theta\right)\chi^{(\gamma)} - B_{\gamma\gamma'} , \quad \text{(A19)}$$

$$B_{\gamma\gamma'} = \int_0^T dt\int_0^T ds\,\chi^{(\gamma)}_{(t)}\Phi(t,s)\chi^{(\gamma')}(s) , \quad \text{(A20)}$$

$$C_{\gamma\gamma'} = \int_0^T dt\,\chi^{(\gamma')}\left(\Gamma\frac{d}{dt}-\Theta\right)\chi^{(\gamma)} + B_{\gamma'\gamma} . \quad \text{(A21)}$$

Rewriting Eq. (A18) as

$$\Omega = -\det\begin{pmatrix}A+B & B\\ -B^T+C-A-B & C-B\end{pmatrix} , \quad \text{(A22)}$$

we easily see that

$$\Omega = -\left[\det\int_0^T dt\,\chi^{(\gamma')}\left(\Gamma\frac{d}{dt}-\Theta\right)\chi^{(\gamma)}\right]^2 \quad \text{(A23)}$$

and therefore

$$P^{(N)}_{(R,P)} = \frac{1}{2\pi T}\prod_{\gamma=1}^{N}\varphi_\gamma\left|\det\int_0^T dt\,\chi^{(\gamma')}\left(\Gamma\frac{d}{dt}-\Theta\right)\chi^{(\gamma)}\right|^{-1} . \quad \text{(A24)}$$

We now prove the identity of the right-hand side of Eqs. (A24) and (4.2) for $N\to\infty$. We use a technique used in Ref. 8 and compare the expressions

$$f(\alpha) = -2\pi T\prod_{\gamma=1}^{\infty}\frac{1}{\varphi_\gamma}\det\int_0^T dt\,\chi^{(\gamma')}\left(\Gamma\frac{d}{dt}-\Theta\right)\chi^{(\gamma)} \quad \text{(A25)}$$

and

$$\bar{f}(\alpha) = 2\pi x(\alpha, T) \quad \text{(A26)}$$

as functions of the parameter α which can vary from 0 to 1. We have to prove that f and $\bar{f}$ are identical in absolute value at $\alpha = 1$. In Eq. (A25), $x(\alpha; T)$ is the upper component of the solution of

$$\left(\Gamma\frac{d}{dt} - \alpha\Theta\right)\xi(\alpha,t) = 0 , \qquad \xi(\alpha,0) = \begin{pmatrix}0\\ 1\end{pmatrix} , \qquad \xi(\alpha,t) = \begin{pmatrix}x(\alpha,t)\\ y(\alpha,t)\end{pmatrix} . \quad \text{(A27)}$$

Whenever $\bar{f}(\alpha)$ vanishes, $\xi(\alpha; t)$ can be represented as a linear combination of the $\chi^{(\gamma)}$ and therefore $f(\alpha)$ vanishes, too. The reverse conclusion holds, too.

In particular, both f and $\bar{f}$ vanish at $\alpha = 0$. There, as may be easily proven, also the first derivatives of f and $\bar{f}$ are identical:

$$\left.\frac{df}{d\alpha}\right|_{\alpha=0}=\left.\frac{d\bar{f}}{d\alpha}\right|_{\alpha=0}=\int_0^T dt(0,1)\left(\Gamma\frac{d}{dt}-\Theta\right)\begin{pmatrix}0\\1\end{pmatrix} \qquad (A28)$$

and in general nonvanishing.

Therefore, in order to prove the identity of f and $\bar{f}$ at $\alpha=1$, it is sufficient to compare the logarithmic derivatives whenever f and $\bar{f}$ are nonvanishing.

With the notation

$$D_{\gamma\gamma'}(\alpha)=\int_0^T dt\,\chi^{(\gamma')}\left(\Gamma\frac{d}{dt}-\alpha\Theta\right)\chi^{(\gamma)}\ , \qquad (A29)$$

$$D(\alpha)=\det D_{\gamma\gamma'}(\alpha)\ , \qquad (A30)$$

and $d_{\gamma\gamma'}^{(\alpha)}$ the (γ,γ') minor of $D(\alpha)$ we obtain

$$\frac{1}{f(\alpha)}\frac{d}{d\alpha}f(\alpha)=\sum_{\gamma,\gamma'}\frac{1}{D(\alpha)}d_{\gamma\gamma'}(\alpha)\int_0^T dt\,\chi^{(\gamma')}\Theta\chi^{(\gamma)}\ . \qquad (A31)$$

Turning to $\bar{f}(\alpha)$ we need the derivative of $\xi(\alpha,t)$ with respect to α. It satisfies the equation

$$\left(\Gamma\frac{d}{dt}-\Theta\right)\frac{d\xi}{d\alpha}(\alpha,t)=\Theta\,\xi(\alpha,t)\ ,\qquad \frac{d}{d\alpha}\xi(\alpha,0)=\begin{pmatrix}0\\0\end{pmatrix}, \qquad (A32)$$

which may be solved with the ansatz

$$\frac{d}{d\alpha}\xi(\alpha,t)=A(\alpha)\xi(\alpha,t)+\sum_\gamma b_\gamma(\alpha)\chi^{(\gamma)}(t)\ . \qquad (A33)$$

$A(\alpha)$ is the desired logarithmic derivative. Equation (A32) is equivalent to

$$\sum_\gamma b_\gamma(\alpha)D_{\gamma\gamma'}(\alpha)=\int_0^T dt\,\chi^{(\gamma')}\Theta\,\xi(\alpha,t)\ ,$$
$$A(\alpha)+\sum_\gamma b_\gamma(\alpha)[\xi(\alpha,0)\chi^{(\gamma)}(0)]=0\ . \qquad (A34)$$

Solving for $A(\alpha)$, we obtain

$$\frac{1}{\bar{f}(\alpha)}\frac{d}{d\alpha}\bar{f}(\alpha)=\sum_{\gamma,\gamma'}\frac{1}{D(\alpha)}[\xi(\alpha,0)\chi^{(\gamma)}(0)]d_{\gamma\gamma'}(\alpha)\times\int_0^T dt\,\chi^{(\gamma')}\Theta\,\xi(\alpha,t)\ . \qquad (A35)$$

For the comparison of Eqs. (A31) and (A35) we introduce the Green's function G_α for the boundary value problem,

$$\left(\Gamma\frac{d}{dt}-\alpha\Theta\right)\begin{pmatrix}r\\s\end{pmatrix}=0\ ,\qquad r(0)=r(T)=0\ . \qquad (A36)$$

G can be given in two representations

$$G_\alpha(t,t')=\sum_{\gamma,\gamma'}\chi^{(\gamma')}(t)\frac{d_{\gamma\gamma'}(\alpha)}{D(\alpha)}\chi^{(\gamma)}(t') \qquad (A37)$$

and

$$G_\alpha(t,t')=\hat{\xi}(\alpha,t_>)\frac{1}{N}\xi(\alpha,t_<)\ . \qquad (A38)$$

In Eq. (A38), $t_>(t_<)$ is the larger (smaller) of the two arguments t and t', $\hat{\xi}$ is the solution of the integrodifferential equation (A27) with the final condition

$$\hat{\xi}(\alpha,T)=\begin{pmatrix}0\\1\end{pmatrix}\ . \qquad (A39)$$

N is a proper normalization.

Inserting Eq. (A37) into (A31) and (A35) we obtain

$$\frac{1}{f(\alpha)}\frac{df(\alpha)}{d\alpha}=\int_0^T dt\,\Theta G_\alpha(t,t) \qquad (A40)$$

and

$$\frac{1}{\bar{f}(\alpha)}\frac{d\bar{f}(\alpha)}{d\alpha}=\int_0^T dt[G_\alpha(t,0)\xi(\alpha,0)]^T\Theta\,\xi(\alpha,t)\ . \qquad (A41)$$

With the help of Eq. (A38) both expressions can be rewritten as

$$\frac{1}{f(\alpha)}\frac{d}{d\alpha}f(\alpha)=\frac{1}{\bar{f}(\alpha)}\frac{d}{d\alpha}\bar{f}(\alpha)=\frac{1}{N}\int_0^T dt\,\hat{\xi}(\alpha,t)\Theta\,\xi(\alpha,t)\ . \qquad (A42)$$

This completes the proof of Eq. (4.2).

APPENDIX B

In this Appendix, we derive the uniform approximation (4.3)–(4.6) for the inclusive probability when there are two contributing classical trajectories $Q_1(t)=[R_1(t),P_1(t)]$ and $Q_2(t)=[R_2(t),P_2(t)]$. We follow closely the lines of Ref. 7, Appendix C. A general discussion of the uniformization of path integrals may be found in Ref. 8.

We again use the path expansion scheme introduced in Appendix A. With a reference path $Q_0(t)$ every path $[R(t),P(t)]$ contributing to the integral (2.11) can be written as

$$\begin{pmatrix}R(t)\\P(t)\end{pmatrix}=Q_0(t)+\sum_{\gamma=0}^{\infty}\alpha_\gamma\chi^{(\gamma)}(t)\ . \qquad (B1)$$

The functions $\chi^{(\gamma)}(t)$ are discussed in Appendix A. A similar expansion holds for the paths $[\tilde{R}(t),\tilde{P}(t)]$. The path integral (2.11) is now an integral over all the expansion coefficients. We first consider the Nth approximant

$$P^{(N)}=\int\sum_{\gamma=0}^{N}da_\gamma\,d\tilde{a}_\gamma J_N\exp[iS_{\rm eff}^{(N)}(\{a_\gamma,\tilde{a}_\gamma\})]\ , \qquad (B2)$$

which results from truncating the expansion (B1) at $\gamma=N$. In Eq. (B2) the effective action still depends parametrically upon the reference paths $Q_0(t)$ and $\tilde{Q}_0(t)$. The Jacobian J_N is given in Appendix A.

We introduce new variables such that the effective action reads

$$S_{\rm eff}^{(N)}(\{a_\gamma,\tilde{a}_\gamma\})\hat{=}\Psi^{(N)}(u,\tilde{u},\{v_\gamma,\tilde{v}_\gamma\})=\tfrac{1}{3}u^3-\xi u-\tfrac{1}{3}\tilde{u}^3+\xi\tilde{u}+i\eta(u-\tilde{u})^2+\sum_{\gamma=1}^{N}\frac{1}{2}(v_\gamma^2-\tilde{v}_\gamma^2)\ . \qquad (B3)$$

Ψ is the simplest analytical form which is topologically equivalent to $S_{\rm eff}$: In all but two variables Ψ is a quadratic form. It has the same symmetry properties as S_{eff}, namely its real (imaginary) part is odd (even) under the interchange of the two paths Q_1 and Q_2 (as long as the paths are real valued). For $\eta\neq 0$ Ψ exhibits two real and two complex stationary points. The coefficients ξ and η should be fixed by matching the stationary points of the two functions $S_{\rm eff}$ and Ψ upon each other. In the present case two stationary points correspond to complex classical trajectories. Their contribution to the inclusive probability is in general exponentially small. This may allow to map only the two real-valued stationary points

$$(u_1, \tilde{u}_1) \triangleq (\sqrt{\xi}, \sqrt{\xi}) \,\hat{=}\, (Q_1, Q_1)\;, \qquad (u_2, \tilde{u}_2) \triangleq (-\sqrt{\xi}, -\sqrt{\xi}) \,\hat{=}\, (Q_2, Q_2)\;, \tag{B4}$$

and postulate in addition

$$(u_3, \tilde{u}_3) \triangleq (\sqrt{\xi}, -\sqrt{\xi}) \,\hat{=}\, (Q_1, Q_2)\;, \qquad (u_4, \tilde{u}_4) \triangleq (-\sqrt{\xi}, \sqrt{\xi}) \,\hat{=}\, (Q_2, Q_1)\;. \tag{B5}$$

We note that when the complex stationary points happen to be near the real axis they almost coincide with the points taken into account by (B5). The right-hand side of Eqs. (B4) and (B5) represent pairs of trajectories in the double path integral. On the left-hand side we only denote the values for the variables u and $\tilde{u}$ and drop the trivial conditions $v_\gamma = \tilde{v}_\gamma = 0$.

Requiring that at the four points Eq. (B3) holds exactly, we identify the parameters ξ and η to be

$$\xi = [\tfrac{3}{8}(S_{\text{eff}}(Q_2; Q_1) - S_{\text{eff}}(Q_1; Q_2))]^{2/3}\;, \qquad \eta = \frac{1}{8i}\, \xi^{-1}(S_{\text{eff}}(Q_2; Q_1) + S_{\text{eff}}(Q_1, Q_2))\;. \tag{B6}$$

Substituting the new variables into the integral (B2), we get

$$P^{(N)} = \int du\, d\tilde{u} \prod_{\gamma=1}^{N} dv_\gamma\, d\tilde{v}_\gamma \hat{J}_N \exp(i\Psi^{(N)})\;, \tag{B7}$$

$$\hat{J}_N = J_N \frac{\partial(\{a_\gamma, \tilde{a}_\gamma\})}{\partial(u, \tilde{u}, \{v_\gamma, \tilde{v}_\gamma\})}\;. \tag{B8}$$

$\hat{J}_N$ contains the Jacobian of the transformation.

The uniform approximation is achieved by approximating $\hat{J}_N$ by a linear form in u and $\tilde{u}$ in such a way that its actual value is reproduced at those points which dominantly contribute to the integral. These are the stationary points and consistently with our above approximation we consider only the real-valued ones.

At a stationary point the Jacobian of the transformation of variables is given via the second derivatives of the functions S_{eff} and Ψ:

$$\frac{\partial(\{a_\gamma, \tilde{a}_\gamma\})}{\partial(u, \tilde{u}, \{v_\gamma, \tilde{v}_\gamma\})} = \left(\frac{\det \delta^2 \Psi^{(N)}}{\det \delta^2 S_{\text{eff}}^{(N)}}\right)^{1/2}\;, \tag{B9}$$

with

$$\det \delta^2 \Psi^{(N)} = -4u\tilde{u}(-1)^N \tag{B10}$$

and

$$(\det \delta^2 S_{\text{eff}}^{(N)})^{-1/2} = P_{(Q_i)}^{(N)} \frac{i}{(2\pi)^{N+1}} J_N^1\;. \tag{B11}$$

Equation (B11) follows directly from Eq. (A15).

With the ansatz

$$\hat{J}_N \cong \frac{1}{(2\pi)^N} [p + q(u + \tilde{u})]\;, \tag{B12}$$

the exact value of $\hat{J}_N$ at the stationary points are reproduced (for $N \to \infty$) when

$$p = \frac{1}{2\pi}(P_{(Q_1)} + P_{(Q_2)})\;, \qquad q = \frac{1}{\pi}\sqrt{\xi}(P_{(Q_1)} - P_{(Q_2)})\;. \tag{B13}$$

Substituting Eq. (B12) into (B7), we perform the integration over $(u + \tilde{u})$ and obtain finally,

$$P = (P_{(Q_1)} + P_{(Q_2)})\; \frac{|\xi|}{\pi} \int_0^\infty \frac{dx}{\sqrt{x}} \exp(-\eta x^2) \cos\left(\frac{x^3}{12} - \xi x + \frac{\pi}{4}\right). \tag{B14}$$

A contour plot of the integral on the right-hand side is given in Fig. 1.

So far, we restricted ourselves to real-valued classical trajectories and could only calculate the "bright" side of the focus $\xi > 0$. We may, however, provide approximate expressions for the "shadow" side by a proper expansion around the focus. Such a procedure is well known for the conventional Airy uniformization.[14]

Consider the final coordinate $R(T)$ as a function of the initial momentum $P(0)$ and assume a focus at $\bar{P}(0)$

$$\frac{\partial \bar{R}(T)}{\partial \bar{P}(0)} = 0\;. \tag{B15}$$

For definiteness assume $\bar{R}(T)$ to be a maximum. Asking for transitions to values of $R(T)$ larger than $\bar{R}(T)$ the corresponding values of $P(0)$ are complex. Expanding around the focus we find

$$P(0) = \bar{P}(0) \pm i\left[2(R(T) - \bar{R}(T)) \Big/ \left|\frac{\partial^2 \bar{R}(T)}{\partial \bar{P}(0)^2}\right|\right]^{1/2} \tag{B16}$$

and the classical probability along the corresponding trajectories

$$P = \frac{1}{2\pi}\left[2(R(T) - \bar{R}(T)) \left|\frac{\partial^2 \bar{R}(T)}{\partial^2 \bar{P}(0)}\right|\right]^{-1/2}\;. \tag{B17}$$

For the calculation of the parameters ξ and η, we also expand the effective action (2.12) around the focus. It turns out that we have to go up to third order in $[P(0) - \bar{P}(0)]$. The derivatives involved are

$$\frac{\partial S_{\text{eff}}}{\partial P_1(0)} = -\frac{\partial S_{\text{eff}}}{\partial P_2(0)} = \bar{P}(T) \frac{\partial \bar{R}(T)}{\partial \bar{P}(0)} = 0\;, \tag{B18}$$

$$\frac{\partial^2 S_{\text{eff}}}{\partial P_1(0)^2} = \bar{P}(T) \frac{\partial^2 \bar{R}(T)}{\partial \bar{P}(0)^2} + i \sum_{n=1}^{\infty} \frac{\partial}{\partial P_1}\left(\frac{\langle \bar{\varphi}_0 | \varphi_n \rangle_T}{\langle \bar{\varphi}_0 | \varphi_0 \rangle_T}\right) \int_0^T dt \langle \varphi_n | \frac{\partial H}{\partial \bar{P}(0)} | \varphi_0 \rangle_t\;. \tag{B19}$$

Inspecting the contour plot in Fig. 1 for the shadow side of the focus $\xi < 0$ we find that the expression (B14) is almost independent of the parameter η. We conclude that the degree by which condition (3.9) is violated only slightly affects the probability for forbidden transitions. Therefore, we neglect the second term on the right-hand side of Eq. (B19) which relates to the interference condition (3.9). Consistently, the other derivatives of S_{eff} become

$$\frac{\partial^2 S_{\text{eff}}}{\partial P_2(0)^2} = -\frac{\partial^2 S_{\text{eff}}}{\partial P_1(0)^2}\;, \tag{B20}$$

$$\frac{\partial^2 S_{eff}}{\partial P_1(0)\partial P_2(0)} = \frac{\partial^3 S_{eff}}{\partial P_1(0)^2 \partial P_2(0)} = \frac{\partial^3 S_{eff}}{\partial P_1(0)\partial P_2(0)^2} = 0 \; , \quad \text{(B21)}$$

$$\frac{\partial^3 S_{eff}}{\partial P_1(0)^3} = -\frac{\partial^3 S_{eff}}{\partial P_2(0)^3} = \frac{\partial \bar{P}(T)}{\partial \bar{P}(0)} \frac{\partial^2 \bar{R}(T)}{\partial \bar{P}(0)^2} \; . \quad \text{(B22)}$$

In Eq. (B22), we neglect the third derivative of $\bar{R}(T)$ with respect to $\bar{P}(0)$ as was done in the expansion with which we started. Substituting the expansion of S_{eff} into Eq. (B6) we get

$$\xi = -\tfrac{1}{2}(R(T) - \bar{R}(T)) \left(\frac{\partial \bar{P}(T)}{\partial \bar{P}(0)} \left| \frac{\partial^2 \bar{R}(T)}{\partial \bar{P}(0)^2} \right|^{-1/2} \right)^{2/3} , \quad \text{(B23)}$$

$$\eta = 0 \; .$$

We note that at the focus $\xi^{1/2}$ vanishes to the same order as the classical probabilities (B17) diverge whereas the integral in Eq. (B14) stays finite (cf. Fig. 1).

[1]H. A. Weidenmüller, in *Progress in Particle and Nuclear Physics*, edited by D. Wilkinson (Pergamon, London, 1980); M. Lefort and C. Ngô, Ann. Phys. (Paris) **3**, 5 (1978).
[2]C. F. Giese and W. R. Gentry, Phys. Rev. A **10**, 2156 (1974); *Kinetics of Ion-Molecule Reactions*, edited by P. Ausloos (Plenum, New York, 1979).
[3]S. A. Adelman and J. D. Doll, J. Chem. Phys. **61**, 4242 (1974).
[4]R. P. Feynman and A. R. Hibbs, *Quantum Mechanics and Path Integrals* (McGraw Hill, New York, 1965); R. P. Feynman and F. L. Vernon, Jr., Ann. Phys. **24**, 118 (1963).
[5]P. Pechukas, Phys. Rev. 181, 174 (1969).
[6]C. B. Willis and R. H. Picard, Phys. Rev. A **9**, 1343 (1974).
[7]K. Möhring and U. Smilansky, Nucl. Phys. A **338**, 227 (1980).
[8]S. Levit and U. Smilansky, Ann. Phys. **108**, 165 (1977).
[9]G. D. Billing, Chem. Phys. **9**, 359 (1975).
[10]K. J. McCann and M. R. Flannery, J. Chem. Phys. **63**, 4695 (1975).
[11]H. D. Meyer and W. H. Miller, J. Chem. Phys. **70**, 3215 (1979).
[12]W. H. Miller, Adv. Chem. Phys. **25**, 69 (1974).
[13]D. H. E. Gross, K. Möhring, S. Mukamel, U. Smilansky, and M. Sobel (in preparation).
[14]C. Chester, B. Friedman, and F. Ursell, Proc. Cambridge Philos. Soc. **53**, 599 (1957).