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Caustic problems in quantum mechanics with applications to scattering theory

Cécile DeWitt-Morette
Department of Astronomy and Center for Relativity, The University of Texas, Austin, Texas 78712

Bruce Nelson*
Department of Physics, The University of Utah, Salt Lake City, Utah 84112

Tian-Rong Zhang
Department of Physics and Center for Relativity, The University of Texas, Austin, Texas 78712
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We present a detailed discussion of the semiclassical approximations to path integrals when there exist caustics in the relevant family of classical trajectories. We show carefully how the Airy functions arise from the post-semiclassical approximation of the path integral and interpret the coefficients in the Airy functions in terms of the flow of classical trajectories. Finally, we present a configuration-space path integral for the scattering matrix and extend our discussion of caustics to the case of rainbow scattering.

I. INTRODUCTION

If a quantum system has a classical limit, the semiclassical expansion of its propagator can be expressed in terms of the flow of the classical system.[1] The first-order terms in the semiclassical expansion (the strict WKB approximation) are given by the first-order approximation of the classical flow, namely the Jacobi fields. The second-order terms (the Airy regime) which dominate the expansion when there are caustics (when the Jacobi fields are not linearly independent) are given by the second-order approximations of the classical flow, namely the solutions of the "small disturbances of the small disturbances".[2] To show the role of the classical flow, as opposed to a single classical path, in the semiclassical expansion of a system, we analyze in Sec. II classical physics as the limit of quantum physics. In Sec. III, we compute the second-order terms which keep the amplitudes finite when the "WKB approximation breaks down".

We use a path-integral representation of the propagators in which the integrators[3] are expressed in terms of the Jacobi fields of the system. Thus the calculation of the path integral in expansion of powers of $\hbar^{1/2}$ gives, term by term, the semiclassical expansion:

Terms of order $\hbar^{-1}$ give the phase of the WKB approximation, namely the classical action.

Terms of order $\hbar^{-1/2}$ give no contribution by virtue of the Euler-Lagrange equation.

Terms of order $\hbar^{0}$ give the Van Vleck determinants.

Terms of order $\hbar^{1/2}$ give the Airy regime.

Terms of higher order give the semiclassical expansion to any order desired.

We show how to relate the initial wave function of a quantum system to the particular classical flow which gives the semiclassical expansion. We construct the Jacobi fields which give the probability amplitudes for position-to-position, momentum-to-position, position-to-momentum and momentum-to-momentum transitions.

The momentum-to-momentum transition is nothing but a chapter of scattering theory and is discussed in Sec. IV. The path-integral representation of the S matrix with "Jacobi integrators" gives directly the WKB approximation and the Airy regime; it bypasses the circuitous route of partial-wave expansion followed by stationary-phase approximation for the summation over angular momentum. In particular, we establish the following.

(i) The phase of the WKB scattering amplitude is given in terms of the classical action function computed for a classical path defined by its initial and final momentum (and not by any other boundary conditions).

(ii) The Airy regime is obtained from a single expansion in powers of $\hbar^{1/2}$, rather than from the combination of four expansions used by Ford and Wheeler in their classic paper.[4,5] This calculation completes the original result obtained by Schulman.[6]

(iii) The Airy parameters (scaling and argument) are determined explicitly in terms of Jacobi fields and derivations of the potential.

(iv) The results are valid for any potential $V(r,\theta)$ (not necessarily spherically symmetric) which decreases faster than r^{-1} at infinity. The Coulomb case will be treated elsewhere.

The Jacobi fields which form the backbone of this work are easy to compute if the classical solutions are known. The properties of the Jacobi fields used in this paper are summarized in the Appendix of Ref. 2.

II. CLASSICAL PHYSICS AS THE LIMIT OF QUANTUM PHYSICS.

Let M be the configuration space of a system S defined by a Lagrangian L. We assume that M is an n-dimensional Riemannian manifold with the metric

$$g_{\alpha\beta}(q(t))=\partial^2L(q(t),\dot{q}(t))/\partial\dot{q}^{\alpha}(t)\partial\dot{q}^{\beta}(t)\ , \qquad \alpha=1,\ldots,n\ .$$

Consider the flow of classical paths $\{q(t,a,p_a):a\in N\subset M\}$, where $q(t_a,a,p_a)=a$ and where the initial momenta $p_a=\nabla S_0(a)$ are the derivatives of a given real-valued well-behaved function S_0 on N. In general, this flow generates a local group of transformations $\{\Phi_{t-t_a}: t\in T=[t_a,t_b]\}$,

$$\Phi_{t-t_a}: N\to M \text{ by } a\to q(t,a,p_a) \text{ for } t_a\le t\le t_b \ .$$

Classical physics is the limit of quantum physics in the following sense. If the system is localized in N at time $t=t_a$, then the probability of finding it in $\Phi_t(N)$ at time t tends to 1 as $\hbar$ tends to 0, i.e., if N is the support of the initial wave function ϕ, and if ψ is the wave function of the system, then

$$\int_{\Phi_{t-t_a}(N)} |\psi(t,x)|^2\tau_t(x)=\int_N |\phi(x)|^2\tau(x)=1 \ , \quad (2.1)$$

in the limit $\hbar\to 0$, where $\tau(x)$ is the volume element on M, i.e. $\tau(x)=\sqrt{g(x)}dx^1\wedge\cdots\wedge dx^n$ (with $g=\det g_{\alpha\beta}$, and $\tau_t(q(t,a,p_a))$ is the image of $\tau(a)$ under the transformation Φ_{t-t_a}, i.e.,

$$\tau_t(q(t,a,p_a))=|\det_{\alpha\beta}[\partial q^\alpha(t,a,p_a)/\partial a^\beta]|\,\tau(a) \ . \quad (2.2)$$

The quantity

$$K^\alpha_{(\beta)}(t,t_a)\equiv\partial q^\alpha(t,a,p_a)/\partial a^\beta \quad (2.3)$$

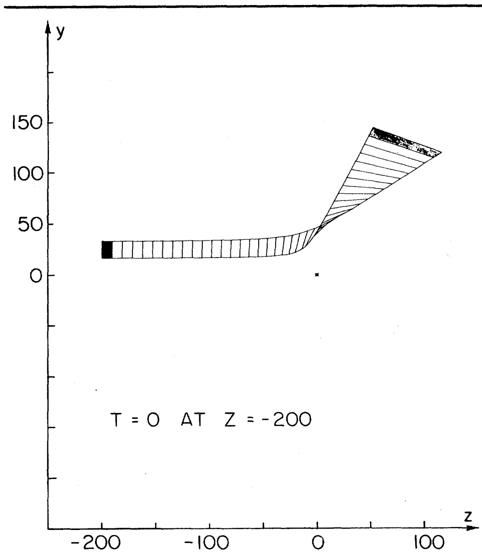

FIG. 1. Consider the flow of Coulomb paths $q(t,B)$ (Figs. 1 and 3) parametrized so that $t=0$ and $z=-200$ for all values of the impact parameter B. Let $h(t,B)$ be the Jacobi field along $q(t,B)$. The particles which, at time $t_a=0$, hit the line element dB defined by the segment of $h(0,B)$ beginning at $q(0,B)$ and ending at $q(0,B+dB)$ hit at time t_b the segment of $h(t_b,B)$ limited by the same classical paths. The integral curve $h(0,B)$ of the Jacobi flow is approximately perpendicular to $q(t,B)$ at $q(0,B)$ because at $z=-200$ the paths are approximately parallel. However, $h(t_b,B)$ is not perpendicular to $q(t,B)$ at $q(t_b,B)$. Thus all the particles hitting dB at t_a do not hit at the same time the exit area, which in the definition of the cross section is assumed to be perpendicular to the classical trajectories. But if we consider the number of particles within the surface of area $v\,dt\,dB$ at time t_a, it is the same as the number of particles within a surface of area $v\,dt\,R\,d\theta$ at time t_b regardless of how slanted the Jacobi fields are at time t_b, and the definition of cross section makes good sense.

defines[2] a Jacobi field $K_{(\beta)}(t,t_a)$ along the classical path $q(t,a,p_a)$ such that $K(t_a,t_a)=\mathbb{1}$. It tells us how the flow $\{q(t,a,p_a): a\in N\}$ diverges or converges (see Fig. 1).

The WKB approximation $\psi_{\rm WKB}$ of the solution ψ of a Schrödinger equation can be defined by

$$\psi=\psi_{\rm WKB}[1+O(\hbar^{1/2})] \ . \quad (2.4)$$

Given a Schrödinger equation and an initial wave function $\phi(x)$,

$$i\hbar\partial\psi/\partial t=H\psi \ ,$$
$$\psi(t_a,x)=\phi(x)=\exp[iS_0(x)/\hbar]T(x) \ , \quad (2.5)$$

where T is an arbitrary well-behaved function on M such that $\operatorname{supp}T=N$, it has been shown that, if $x\in\Phi_{t-t_a}(N)$ and if Φ_{t-t_a} has an inverse, then[7]

$$\psi_{\rm WKB}(t,x)=[\det_{\alpha\beta}K^\alpha_{(\beta)}(t,t_a)]^{-1/2}\times\exp[iS(t,x)/\hbar]T[\Phi_{t-t_a}{}^{-1}(x)] \ , \quad (2.6)$$

where $K^\alpha_{(\beta)}(s,t_a)$ is a Jacobi field along the path $\bar q(s)=\Phi_{s-t_a}\circ\Phi_{t-t_a}{}^{-1}(x)$, and where

$$S(t,x)=S_0(\bar q(t_a))+\int_{t_a}^t L(\bar q(s),\dot{\bar q}(s))ds \ .$$

Hence by virtue of (2.2) and (2.3), $\psi_{\rm WKB}$ satisfies Eq. (2.1), not just in the limit $\hbar\to 0$, but exactly:

$$\int_{\Phi_{t-t_a}(N)} |\psi_{\rm WKB}(t,x)|^2\tau_t(x)=\int_N |T(a)|^2\tau(a) \ . \quad (2.7)$$

It follows that the WKB approximation of the cross section is the classical cross section. Consider a flow of incoming identical particles being scattered by a potential V with compact support K_V and being detected at a distance R from the "center" of the potential, in the direction θ from the incident direction. The scattering cross section $\sigma(\Omega)d\Omega$ in the solid angle $d\Omega(\theta)$ is the ratio of the number of particles hitting the surface area $R^2d\Omega$ per unit time to the number of incident particles per unit area per unit time. The current vector density of a particle of mass m is

$$j=-\frac{i\hbar}{2m}[\psi^*\nabla\psi-(\nabla\psi^*)\psi] \ . \quad (2.8)$$

If we approximate ψ by $\psi_{\rm WKB}$, we obtain

$$j_{\rm WKB}(t,x)=\frac{1}{m}\nabla_x S(t,x)\,|\det_{\alpha\beta}K^{\alpha\beta}(t,t_a)|^{-1}\,|T(a)|^2 \ , \quad (2.9)$$

where t_a is any time before the scattered flux has reached the scatterer, i.e., any time such that

$$j(a)=-\frac{i\hbar}{2m}\{\phi^*(a)\nabla_a\phi(a)-[\nabla_a\phi^*(a)]\phi(a)\}$$
$$=\frac{1}{m}\nabla_a S_0(a)\,|T(a)|^2 \ .$$

For a and x far from the scatterer, the momenta $\nabla_a S_0(a)$ and $\nabla_x\bar S(t,x)$ of the particle are pointing toward, and away from (respectively), the scatterer and

$$\sigma_{\mathrm{WKB}}(\Omega)d\Omega=\frac{|j_{\mathrm{WKB}}(t,x(R,\Omega))|R^2d\Omega}{|j(a)|}$$
$$=|\det_{\alpha\beta}K^{\alpha\beta}(t,t_a)|^{-1}|\nabla S(t,x(R,\Omega))|R^2d\Omega\,|\nabla S_0(a)|^{-1}\,. \tag{2.10}$$

One can rewrite (2.10) in terms of the volume factors τ, and the path $\bar{q}(s)=\Phi_{s-t_a}\circ\Phi_{t-t_a}{}^{-1}(s)$,

$$\sigma_{\mathrm{WKB}}(\Omega)=R^2\frac{\tau(\bar{q}(t_a))}{\tau_t(\bar{q}(t))}\frac{|\nabla S(t,\bar{q}(t))|}{|\nabla S_0(\bar{q}(t_a))|}$$
$$=R^2\text{ (surface area of impact of the flow)/(its surface area of exit)}\,, \tag{2.11}$$

which is precisely the classical cross section.

For an axial symmetric potential in $\mathbf{R}^3$, if we take the surface of impact to be the annulus of area $2\pi B\,dB$, then the exit surface area is $R^2d\Omega\ =R^2\sin\theta\,d\theta\int_0^{2\pi}d\phi$ for $\Omega=(\theta,\phi)$ and

$$\sigma_{\mathrm{WKB}}(\Omega)=B\,dB/\sin\theta\,d\theta\,. \tag{2.12}$$

III. CLASSICAL PHYSICS AS THE LIMIT OF QUANTUM PHYSICS WHEN THE WKB APPROXIMATION BREAKS DOWN

A. Introduction

In the previous section, we have considered flows $\{\Phi_{t-t_a}:t\in T\}$ of classical paths when T is sufficiently small for Φ_{t-t_a} to have an inverse, equivalently for $\det K^{\alpha}{}_{\beta}(t,t_a)$ to be nonvanishing. We now remove this restriction. We are interested in the four following situations:

(i) Final position does not necessarily characterize a unique path in a family of classical paths having the same initial position. For example, a family of catenaries (Fig. 2).

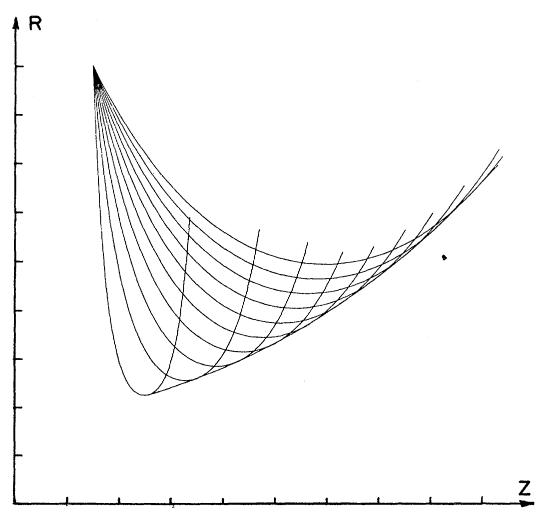

FIG. 2. For x in the "dark side" of the caustic there is no classical path; for x on the "bright side" of the caustic there are two classical paths which coalesce into a single one as x approaches the caustic.

(ii) Final position does not necessarily characterize a unique path in a given classical flow. For example, a family of classical paths having the same initial momentum in a repulsive Coulomb potential (Fig. 3).[8]

(iii) Final momentum does not necessarily characterize a unique path in a family of classical paths having the same initial position. For example, rainbow scattering from a point source (Fig. 4).

(iv) Final momentum does not necessarily characterize a unique path in a given classical flow. For example, rainbow scattering from a source at infinity (Fig. 5).

The first two families of classical paths have an envelope and their study is clearly a caustic problem.[9] Phase-space drawings projected onto momentum space, as opposed to position space, would show that the study of the last two families of classical paths is also a caustic problem: A small variation in the initial momenta (case iii) at time t_a or a small variation in the initial position (case iv) at time t_a produces (for certain values of t) a variation in the final momenta of a smaller order of magnitude; the final momenta are "parallel to first order": There is a direction, say along the α axis, where $\partial\dot{q}(t,a,p_a)/\partial p_{a\alpha}=0$ (case iii) or $\partial\dot{q}(t,a,p_a)/\partial a^{\alpha}=0$ (case iv). In all four cases the criterion for the existence of caustics is the presence of nonzero Jacobi fields $h(t)$ with vanishing boundary conditions:

$$\text{case (i):}\quad h(t_a)=h(t_b)=0\,,$$
$$\text{case (ii):}\quad \dot{h}(t_a)=h(t_b)=0\,,$$
$$\text{case (iii):}\quad h(t_a)=\dot{h}(t_b)=0\,,$$
$$\text{case (iv):}\quad \dot{h}(t_a)=\dot{h}(t_b)=0\,.$$

We shall investigate the transition amplitudes corresponding to these four situations and their limits when $\hbar$ tends to zero. The initial wave function for cases (i) and (iii) is a δ function charging the initial position. The initial wave function[10] for cases (ii) and (iv) corresponding to the flow $p_a=\nabla S_a$ is

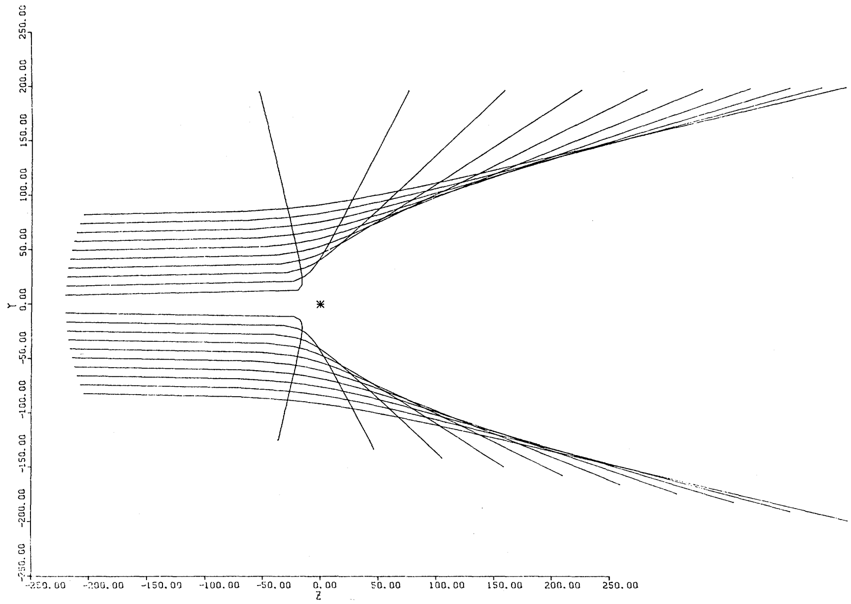

FIG. 3. Let $A \equiv lE/mv_0^2$ and $B \equiv$ impact parameter. The family of Coulomb paths having the same initial momentum is the B family satisfying $B(y-B)=A(z+z^2+y^2)^{1/2}$ in the y-z plane. Its envelope is the parabola $y^2=8A(z+2A)$. For A negative the flow is not caustic forming.

$$\phi=\exp\left[\frac{i}{\hbar}S_a\right]T ,$$

where T satisfies the same conditions as in (2.3).

The transition amplitude for case (i) can be obtained[11] from either Feynman-Kac formulas (A45) or (A46). The transition amplitude for case (ii) can be obtained[1] from the Feynman-Kac formula (A45) and the one for case (iii) from the Feynman-Kac formula (A46). However, since we are interested here in applications to scattering theory, we shall consider transitions from momentum states as $t_a \rightarrow -\infty$ (case ii) and transitions to momentum states as $t_b \rightarrow +\infty$, and use the path-integral representation of the Møller wave operators derived in Ref. 1. Case (iii) can be obtained either as in Ref. 1 by reversing time in the formulas used in case (ii), or from a phase-space path integral.[12] Case (iv) can be obtained either from a phase-space integral[12] or, by relating[13] it to case (ii) when $t_a \rightarrow -\infty$ and $t_b \rightarrow \infty$.

We shall show how the WKB approximations break down in these four cases and how the contribution of the higher-order terms in an expansion in powers of $\hbar^{1/2}$ keep the transition amplitudes finite.

The absolute values squared of the WKB approximations are proportional, respectively, to the following determinants:

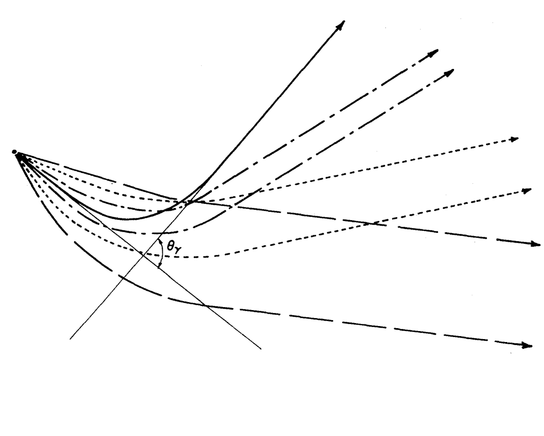

FIG. 4. If the classical deflection function is of the type given in Fig. 2 of Ref. 4, two paths with different angular momentum have the same scattering angles $\theta < \theta_r$. The two paths coalesce at $\theta=\theta_r$. No path is scattered with an angle larger than θ_r.

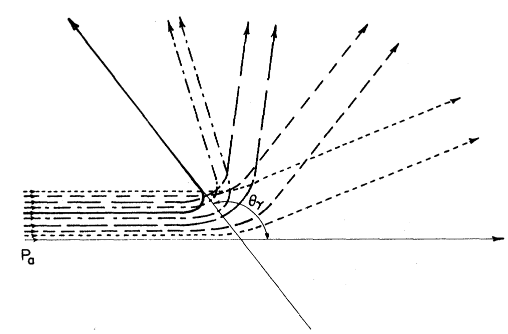

FIG. 5. Rainbow scattering from a source at infinity.

$$\text{case (i):}\quad |\mathscr{K}_{\mathrm{WKB}}(b,t_b;a,t_a)|^2 \sim |\det_{\alpha\beta}\partial q^\alpha(t_b,a,p_a)/\partial p_{a\beta}|^{-1} \equiv |\det_{\alpha\beta} J^{\alpha\beta}(t_b,t_a)|^{-1}\,, \tag{3.1}$$

$$\text{case (ii):}\quad |\mathscr{K}_{\mathrm{WKB}}(b,t_b;p_a,t_a)|^2 \sim |\det_{\alpha\beta}\partial q^\alpha(t_b,a,p_a)/\partial a^\beta|^{-1} \equiv |\det_{\alpha\beta} K^\alpha{}_\beta(t_b,t_a)|^{-1}\,, \tag{3.2}$$

$$\text{case (iii):}\quad |\mathscr{K}_{\mathrm{WKB}}(p_b,t_b;a,t_a)|^2 \sim |\det_{\alpha\beta}\partial p_\alpha(t_b,a,p_a)/\partial p_{a\beta}|^{-1} \equiv |\det_{\alpha\beta} \widetilde{K}_\alpha{}^\beta(t_b,t_a)|^{-1}\,, \tag{3.3}$$

$$\text{case (iv):}\quad |\hat{\mathscr{K}}_{\mathrm{WKB}}(p_b,t_b;p_a,t_a)|^2 \sim |\widehat{\det_{\alpha\beta}}\,\partial p_\alpha(t_b,a,p_a)/\partial a^\beta|^{-1} \equiv |\widehat{\det_{\alpha\beta}}\, L_{\alpha\beta}(t_a,t_b)|^{-1}\,, \tag{3.4}$$

where a caret over a determinant means the truncated determinant equal to the product of the nonzero eigenvalues of the matrix. J and K are the Jacobi matrices[14] constructed from Jacobi fields, and $\widetilde{K}$ and L are derivatives of the Jacobi matrices. The vanishing of their determinants signals the presence of caustics in configuration space ($\det J=0$ or $\det K=0$) or in phase space ($\det\widetilde{K}=0, \widehat{\det} L=0$), since a caustic occurs when the Jacobi fields are not linearly independent. The higher-order terms in the calculation of the transition amplitudes come from path integrals in which the integrator is a Green's function of the Jacobi operator with boundary conditions dictated by the initial and final states of cases (i), (ii), (iii), and (iv), respectively. We shall establish first [Eqs. (3.14), (3.15), (3.22), (3.23), (3.28), (3.29), (3.33), and (3.34), in Sec. III B] basic properties of the zero eigenvalues of the Jacobi operator for the various boundary conditions needed. These properties are used in Sec. III C to compute the probability amplitudes in the Airy regime for cases (i), (ii), and (iii). Another section (Sec. IV) is devoted to case (iv) because the existence of conservation laws in a momentum-to-momentum transition introduces new problems which are analyzed in Ref. 2.

B. Zero eigenvalues of Jacobi operators

An eigenfunction of the Jacobi operator with a zero eigenvalue is also a nonzero Jacobi field with zero boundary conditions. We shall consider the four cases of Dirichlet boundary conditions, von Neumann boundary conditions, and the two sets of mixed boundary conditions. These four cases are sufficiently different to require individual investigation.

(i) Dirichlet boundary conditions.

Let $\mathscr{F}(q)$ be the Jacobi operator of a system, evaluated along the path q. Let $\{\psi_k\}$ be a complete orthogonal set of eigenfunctions of $\mathscr{F}(q)$ with vanishing Dirichlet conditions; i.e.,

$$\mathscr{F}(q)_{\mu\nu}\psi^\nu{}_k(t)=\alpha_k\delta_{\mu\nu}\psi^\nu{}_k(t) \text{ (with no sum over } k)\,,$$
$$\psi_k(t_a)=\psi_k(t_b)=0\,, \tag{3.5}$$

and

$$\int_T (\psi_k(t)\,|\,\psi_j(t))dt=\delta_{kj}\,.$$

We shall gain information about the eigenvalues of $\mathscr{F}(q)$ by comparing two different expressions of its Green's function G. It can be checked that, if there is no zero eigenvalue, then the two expressions for G,

$$G^{\alpha\beta}(t,s)=\sum_k \alpha_k{}^{-1}\psi_k{}^\alpha(t)\psi_k{}^\beta(s) \tag{3.6}$$

and[15]

$$G^{\alpha\beta}(t,s)=\theta(s-t)(J(t,t_a)M(t_a,t_b)J(t_b,s))^{\alpha\beta} - \theta(t-s)(J(t,t_b)M(t_b,t_a)J(t_a,s))^{\alpha\beta} \tag{3.7}$$

(where θ is the step function equal to 1 for positive arguments and zero otherwise) are both solutions of

$$(\mathscr{F}_t(q))_{\alpha\beta}G^{\beta\gamma}(t,s)=\delta_\alpha^\gamma\delta(t-s) \tag{3.8}$$

with the same boundary conditions.

From (3.6) it follows that

$$\alpha_k{}^{-1}=\int_T dt\int_T ds\,\psi_k(t)G(t,s)\psi_k(s)\,, \tag{3.9}$$

where summation of the Greek indices is implied and does not need to be spelled out since the time variable keeps track of the tangent space $T_{q(t)}M$ where the summation occurs.

From (3.7) it follows that

$$\alpha_k{}^{-1}=2\int_T ds\int_T dt\,\theta(s-t)\psi_k(t)J(t,t_a) \times M(t_a,t_b)J(t_b,s)\psi_k(s) \tag{3.10}$$

[where we have used the antisymmetry properties $J^{\alpha\beta}(t,s)=-J^{\beta\alpha}(s,t)$]. If $q(t_a)$ and $q(t_b)$ are conjugate, there is at least one zero eigenvalue and Eq. (3.9) is meaningless. In this case, let q^Δ be a nearby classical path. For instance, q and q^Δ can be solutions of the same Euler-Lagrange equation with slightly different boundary conditions, say

$$q(t_a)=q^\Delta(t_a)=a\,,\quad q(t_b)=b\,,\quad q^\Delta(t_b)=b^\Delta=b+\Delta\,.$$

If a and b are conjugate and a and b^Δ are not conjugate, we shall investigate the caustic by studying the limits of the Jacobi fields along q^Δ when b^Δ tends to b, i.e., when Δ tends to zero. Assume first that there is only one nonzero Jacobi field with vanishing boundary conditions, say $\psi_{(1)}$. Then $\psi_{(1)}(t)$ can be written in terms of its boundary values and the Jacobi matrices:

$$\psi_{(1)}(t)=J(t,t_a)\dot{\psi}_{(1)}(t_a)=-\dot{\psi}_{(1)}(t_b)J(t_b,t)\,. \tag{3.11}$$

Let J^Δ be the Jacobi matrix corresponding to q^Δ, and let $\{a^\Delta{}_k\}$ and $\{\psi^\Delta{}_k\}$ be the eigenvalues and eigenfunctions of $\mathscr{F}(q^\Delta)$. It is possible to choose a coordinate system which block diagonalizes the matrix $J^\Delta(t_b,t_a)$ into a block whose determinant vanishes when $\Delta=0$ and one which does not. In this frame of reference,

$$J^\Delta(t_b,t_a)=\begin{bmatrix}\epsilon & 0\\ 0 & \hat{J}^\Delta(t_b,t_a)\end{bmatrix}\,,$$

$$M^\Delta(t_a,t_b)=\begin{bmatrix}\epsilon^{-1} & 0\\ 0 & \hat{M}^\Delta(t_a,t_b)\end{bmatrix}$$

and Eq. (3.10) can be written

$$(\alpha_1^\Delta)^{-1}=2\int_T ds\int_T dt\,\theta(s-t)\psi^\Delta_{(1)\alpha}(t)J^{\Delta\alpha}{}_1(t,t_a)M^{\Delta 1}{}_1(t_a,t_b)J^{\Delta 1}{}_\beta(t_b,s)\psi^{\Delta\beta}_{(1)}(s)+\text{ terms of order }\epsilon^0\,. \tag{3.12}$$

On the other hand,

$$\begin{aligned}\lim_{\Delta\to 0}J^{\Delta\alpha}{}_1(t,t_a)&=J^\alpha{}_1(t,t_a)\\&=\psi^\alpha_{(1)}(t)/\dot\psi^1_{(1)}(t_a)\,,\\\lim_{\Delta\to 0}J^{\Delta 1}{}_\beta(t_b,s)&=J^1{}_\beta(t_b,s)\\&=\psi_{(1)\beta}(s)/\dot\psi_{(1)1}(t_b)\,.\end{aligned}\tag{3.13}$$

Indeed,

$$\dot\psi_{(1)}(t_a)=M(t_a,t)\psi_{(1)}(t)$$

and

$$\dot\psi^\alpha_{(1)}(t_a)=\lim_{\Delta\to 0}M^{\Delta\alpha}_\beta(t_a,t)\psi^\beta_{(1)}(t)\,.$$

This last equation remains true as t tends to t_b. Thus in the chosen system of coordinates where $M^{\Delta 1}{}_1(t_a,t_b)$ is the dominant component, $\dot\psi^\alpha_{(1)}(t_a)$ has only one nonzero component $\dot\psi^1_{(1)}(t_a)$ and

$$\psi^\alpha_{(1)}(t)=J^\alpha{}_1(t,t_a)\dot\psi^1{}_{(1)}(t_a)\,.$$

The second part of Eq. (3.13) is proved similarly. Substituting (3.13) into (3.12) and using the orthonormal condition (3.5) gives

$$\lim_{\Delta\to 0}(\alpha_1^\alpha)^{-1}=\lim_{\Delta\to 0}M^{\Delta 1}{}_1(t_a,t_b)/\dot\psi^1_{(1)}(t_a)\dot\psi_{(1)1}(t_b)$$

and (3.14)

$$\lim_{\Delta\to 0}(\alpha_1^\Delta)^{-1}\det J^\Delta(t_b,t_a)=\det\hat J(t_b,t_a)/\dot\psi^1{}_{(1)}(t_a)\dot\psi_{(1)1}(t_b)\,.$$

If there is more than one nonzero Jacobi field with vanishing boundary conditions, say $\psi_{(1)},\dots,\psi_{(j)}$, a similar analysis gives

$$\lim_{\Delta\to 0}(\alpha_1^\Delta\cdots\alpha_j^\Delta)^{-1}\det J^\Delta(t_b,t_a)=\det\hat J(t_b,t_a)\Big/\prod_{i=1}^{j}\dot\psi^i{}_{(i)}(t_a)\dot\psi_{(i)i}(t_b)\,,\tag{3.15}$$

where $\hat J(t_b,t_a)$ is the truncated matrix obtained from $J(t_b,t_a)$ by removing the first j columns and j rows in the system of coordinates which block diagonalizes J into a block whose determinant vanishes when $\Delta=0$, and one which does not

$$J^\Delta(t_b,t_a)=\begin{bmatrix}(j\times j) & 0\\ \text{matrix} & \\ 0 & \hat J^\Delta(t_b,t_a)\end{bmatrix}.$$

Equation (3.15) shows how zero eigenvalues of the Jacobi operator combine with Jacobi fields to give a finite expression.

(ii) Mixed boundary conditions.

Let $\{\psi_k\}$ be a complete orthogonal set of eigenfunctions of $\mathscr{F}(q)$ with vanishing mixed conditions

$$\dot\psi_k(t_a)=\psi_k(t_b)=0\,.$$

The Green's function of $\mathscr{F}(q)$ corresponding to these boundary conditions is[15]

$$\begin{aligned}G_+(t,s)=\;&\theta(s-t)K(t,t_a)N(t_a,t_b)J(t_b,s)\\&-\theta(t-s)J(t,t_b)\tilde N(t_b,t_a)\tilde K(t_a,s)\,.\end{aligned}\tag{3.16}$$

The Jacobi K matrix has no symmetry property, hence the appearance of the transpose matrix $\tilde K$ and its inverse. Inserting (3.16) into (3.9) gives

$$\begin{aligned}\alpha_k{}^{-1}=2\int_T ds\int_T dt\,\theta(s-t)\psi_k(t)K(t,t_a)\\\times N(t_a,t_b)J(t_b,s)\psi_k(s)\,.\end{aligned}\tag{3.17}$$

Again if the family of classical paths with given initial velocities is caustic forming and if $q(t_b)=b$ is on the caustic, then there is at least one zero eigenvalue and Eq. (3.6) is meaningless. We shall proceed as before and introduce a nearby classical path q^Δ satisfying the same Euler equation as q but different boundary conditions, namely

$$\begin{aligned}&\dot q(t_a)=\dot q^\Delta(t_a)=v_a\,,\quad q(t_b)=b\,,\\&q^\Delta(t_b)=b^\Delta=b+\Delta\,.\end{aligned}$$

Assume first that there is only one nonzero Jacobi field with vanishing boundary conditions, say $\psi_{(1)}$. Then

$$\begin{aligned}\psi_{(1)}(t)&=K(t,t_a)\psi_{(1)}(t_a)\\&=\dot\psi_{(1)}(t_b)J(t_b,t)\,.\end{aligned}\tag{3.18}$$

Let K^Δ be the Jacobi matrix corresponding to q^Δ, and choose a frame of reference which block diagonalizes $K^\Delta(t_b,t_a)$ into a block whose determinant vanishes when $\Delta=0$, and one which does not:

$$K^\Delta(t_b,t_a)=\begin{bmatrix}\epsilon & 0\\ 0 & \hat K^\Delta(t_b,t_a)\end{bmatrix},$$

$$N^\Delta(t_a,t_b)=\begin{bmatrix}\epsilon^{-1} & 0\\ 0 & \hat N^\Delta(t_a,t_b)\end{bmatrix}.$$

Hence

$$(\alpha_1^\Delta)^{-1}=2\int_T ds\int_T dt\,\theta(s-t)\psi^\Delta_{(1)\alpha}(t)K^{\Delta\alpha}{}_1(t,t_a)N^{\Delta 1}{}_1(t_a,t_b)J^{\Delta 1}{}_\beta(t_b,s)\psi^{\Delta\beta}_{(1)}(s)\,.\tag{3.19}$$

On the other hand,

$$\lim_{\Delta\to 0} K^{\Delta\alpha}{}_1(t,t_a)=K^{\alpha}{}_1(t,t_a)=\psi^{\alpha}_{(1)}(t)/\psi^{1}_{(1)}(t_a)\,, \tag{3.20}$$

$$\lim_{\Delta\to 0} J^{\Delta 1}{}_{\beta}(t_b,t)=J^{1}{}_{\beta}(t_b,t)=\psi_{(1)\beta}(t)/\dot{\psi}_{(1)1}(t_b)\,. \tag{3.21}$$

Equation (3.20) is proved like Eqs. (3.13). To prove Eq. (3.21), note that[16] $\dot{J}(t,t_a)=\tilde{K}(t,t_a)$. Hence

$$\begin{aligned}\dot{\psi}_{(1)\alpha}(t)&=\dot{\psi}_{(1)\beta}(t_b)\dot{J}^{\beta}{}_{\alpha}(t_b,t)\\&=\dot{\psi}_{(1)\beta}(t_b)\dot{J}_{\alpha}{}^{\beta}(t,t_b)\\&=\dot{\psi}_{(1)1}(t_b)K^{\beta}{}_{\alpha}(t_b,t)\end{aligned}$$

and by the same argument as before, in the chosen system of coordinates $\dot{\psi}_{(1)}(t_b)$ has only one nonzero component $\dot{\psi}_{(1)1}(t_b)$. Equation (3.21) follows from Eq. (3.18). Finally, substituting (3.20) and (3.21) in (3.19), and using the orthonormal condition (3.5) gives

$$\lim_{\Delta\to 0}(\alpha_1^{\Delta})^{-1}\det K^{\Delta}(t_b,t_a)=\det\hat{K}(t_b,t_a)/\psi^{1}_{(1)}(t_a)\dot{\psi}_{(1)1}(t_b)\,. \tag{3.22}$$

If there is more than one nonzero Jacobi field with vanishing boundary conditions, say $\psi_{(1)},\ldots,\psi_{(j)}$, a similar analysis gives

$$\lim_{\Delta\to 0}(\alpha_1^{\Delta}\cdots\alpha_j^{\Delta})^{-1}\det K^{\Delta}(t_b,t_a) =\det\hat{K}(t_b,t_a)\Big/\prod_{i=1}^{j}\psi^{i}_{(i)}(t_a)\dot{\psi}_{(i)i}(t_b)\,. \tag{3.23}$$

(iii) Mixed boundary conditions.

Let $\{\psi_k\}$ be a complete orthonormal set of eigenfunctions of $\mathscr{F}(q)$ with vanishing mixed boundary conditions: $\psi_k(t_a)=\dot{\psi}_k(t_b)=0$. The Green's function of $\mathscr{F}(q)$ corresponding to these boundary conditions is[15]

$$\begin{aligned}G(t,s)=&\ \theta(s-t)J(t,t_a)\tilde{N}(t_a,t_b)\tilde{K}(t_b,s)\\&-\theta(t-s)K(t,t_b)N(t_b,t_a)J(t_a,s)\,.\end{aligned} \tag{3.24}$$

Inserting this expression of the Green's function into (3.9) gives

$$\begin{aligned}\alpha_k{}^{-1}=2\int_T ds\int_T dt\,\theta(s-t)\psi_k(t)J(t,t_a)&\\ \times\tilde{N}(t_a,t_b)\tilde{K}(t_b,s)\psi_k(s)\,.&\end{aligned} \tag{3.25}$$

We shall again introduce a nearby classical path q^{Δ} satisfying the same Euler equation as q but different boundary conditions at t_b, namely

$$\begin{aligned}&q(t_a)=q^{\Delta}(t_a)=a\,,\\&\dot{q}(t_b)=r_b\,,\\&\dot{q}^{\Delta}(t_b)=r^{a}{}_{b}=r_b+\Delta\,.\end{aligned} \tag{3.26}$$

Note that Δ is a variation in velocity, in contrast to the first two cases where Δ is a variation in position.

Assume first that there is only one Jacobi field with vanishing boundary conditions, say $\psi_{(1)}(t)$. Then $\psi_{(1)}(t)=J(t,t_a)=\dot{\psi}_{(1)}(t_b)\tilde{K}(t_b,t)$.

Let $\tilde{K}^{\Delta}$ be the matrix corresponding to q^{Δ}, and let us choose a frame of reference where

$$\tilde{K}^{\Delta}(t_b,t_a)=\begin{bmatrix}\epsilon & 0\\ 0 & \hat{\tilde{K}}^{\Delta}(t_b,t_a)\end{bmatrix},$$

$$\tilde{N}^{\Delta}(t_a,t_b)=\begin{bmatrix}\epsilon^{-1} & 0\\ 0 & \hat{\tilde{N}}^{\Delta}(t_a,t_b)\end{bmatrix}.$$

Then the singular eigenvalue of $\mathscr{F}$ can be written as

$$\begin{aligned}(\alpha_1^{\Delta})^{-1}=2\int_T ds\int_T dt\,\theta(s-t)\psi^{\Delta}_{(1)\alpha}(t)J^{\Delta\alpha 1}(t,t_a)&\\ \times\tilde{N}^{\Delta 1}{}_{1}(t_a,t_b)\tilde{K}_1^{\Delta\beta}(t_b,s)\psi^{\Delta}_{(1)\beta}(s)\,.&\end{aligned} \tag{3.27}$$

On the other hand,

$$\lim_{\Delta\to 0}J^{\Delta\alpha 1}(t,t_a)=J^{\alpha 1}(t,t_a)=\psi^{\alpha}_{(1)}(t)/\dot{\psi}_{(1)1}(t_a)\,,$$

$$\lim_{\Delta\to 0}\tilde{K}^{\Delta\beta}{}_{1}(t_b,s)=\tilde{K}_1{}^{\beta}(t_b,s)=\psi^{\beta}_{(1)}(s)/\psi^{1}_{(1)}(t_b)\,.$$

Substituting these expressions in (3.27) and using the orthonormal condition (3.5) gives

$$\lim_{\Delta\to 0}(\alpha_1^{\Delta})^{-1}\det\tilde{K}^{\Delta}(t_b,t_a)=\det\hat{\tilde{K}}(t_b,t_a)/\dot{\psi}_{(1)1}(t_a)\psi^{1}_{(1)}(t_b)\,. \tag{3.28}$$

If there is more than one nonzero Jacobi field with boundary conditions, say $\psi_{(1)},\ldots,\psi_{(j)}$, a similar analysis gives

$$\lim_{\Delta\to 0}(\alpha_1^{\Delta}\cdots\alpha_j^{\Delta})^{-1}\det\tilde{K}^{\Delta}(t_b,t_a) =\det\hat{\tilde{K}}(t_b,t_a)\Big/\prod_{i=1}^{j}\dot{\psi}_{(i)}(t_a)\psi_{(i)}(t_b)\,. \tag{3.29}$$

(iv) Neumann boundary conditions.

Let $\{\psi_k\}$ be a complete orthonormal set of eigenfunctions of $\mathscr{F}(q)$ with vanishing von Neumann conditions

$$\dot{\psi}_k(t_a)=\dot{\psi}_k(t_b)=0\,.$$

The Green's function of $\mathscr{F}(q)$ corresponding to these boundary conditions is[2]

$$\begin{aligned}G(t,s)=&\ \theta(s-t)K(t,t_a)P(t_a,t_b)\tilde{K}(t_b,s)\\&+\theta(t-s)K(t,t_b)\tilde{P}(t_b,t_a)\tilde{K}(t_a,s)\,,\end{aligned} \tag{3.30}$$

where $P(t,t_a)$ is the inverse of $\dot{K}(t,t_a)$. Inserting this expression of the Green's function into (3.9) gives

$$\begin{aligned}\alpha_k{}^{-1}=2\int_T ds\int_T dt\,\theta(s-t)\psi_k(t)K(t,t_a)&\\ \times P(t_a,t_b)\tilde{K}(t_b,s)\psi_k(s)\,.&\end{aligned} \tag{3.31}$$

The occurrence of zero eigenvalues makes Eq. (3.6) meaningless, and we shall again introduce a nearby classical path q^{Δ} satisfying the same Euler equation as q but different boundary conditions at t_b, namely

$$\begin{aligned}&\dot{q}(t_a)=\dot{q}^{\Delta}(t_a)=v_a\,,\\&\dot{q}(t_b)=v_b\,,\\&\dot{q}^{\Delta}(t_b)=v_b^{\Delta}=v_b+\Delta\,.\end{aligned} \tag{3.32}$$

We assume that the Jacobi field along q has vanishing Neumann boundary conditions, but the Jacobi field along

q^Δ does not. Assume first that there is only one Jacobi field with vanishing boundary conditions, say $\psi_{(1)}$. Then

$$\psi_{(1)}(t)=K(t,t_a)\psi_{(1)}(t_a)=\psi_{(1)}(t_b)\tilde{K}(t_b,t)\ .$$

Let

$$L^\Delta(t_b,t_a)=\nabla_{t_b}K^\Delta(t_b,t_a)$$

be the matrix corresponding to q^Δ, and choose a frame of reference where

$$L^\Delta(t_b,t_a)=\begin{bmatrix}\epsilon & 0\\ 0 & \hat{L}^\Delta(t_b,t_a)\end{bmatrix}\ ,$$

$$P^\Delta(t_a,t_b)=\begin{bmatrix}\epsilon^{-1} & 0\\ 0 & \hat{P}^\Delta(t_a,t_b)\end{bmatrix}\ .$$

Hence

$$(\alpha_1^\Delta)^{-1}=2\int_T ds\int_T dt\,\theta(s-t)\psi^\Delta_{(1)\alpha}(t)K^{\Delta\alpha}{}_1(t,t_a)\times P^{\Delta 1}{}_1(t_a,t_b)\tilde{K}^{\Delta 1}{}_\beta(t_b,s)\psi^{\Delta\beta}_{(1)}(s)\ .$$

And by virtue of equations (3.20) and (3.29), together with the orthonormality relation of the eigenfunctions,

$$\lim_{\Delta\to 0}(\alpha_1^\Delta)^{-1}=\lim_{\Delta\to 0}P^{\Delta 1}{}_1(t_a,t_b)/\psi_{(1)}(t_a)\psi_{(2)}(t_b)\ ,$$
$$\lim_{\Delta\to 0}(\alpha_1^\Delta)^{-1}\det L^\Delta(t_b,t_a)=\det\hat{L}(t_b,t_a)/\psi_{(1)}(t_a)\psi_{(1)}(t_b)\ . \tag{3.33}$$

If there is more than one zero Jacobi field with vanishing boundary conditions, say $\psi_{(1)},\dots,\psi_{(k)}$, a similar analysis gives

$$\lim_{\Delta\to 0}(\alpha_1^\Delta\cdots\alpha_k^\Delta)^{-1}\det L^\Delta(t_b,t_a)=\det\hat{L}(t_b,t_a)\Big/\prod_{i=1}^{k}\psi_i(t_a)\psi_i(t_b)\ , \tag{3.34}$$

where $\hat{L}$ is the appropriate truncated matrix similar to (3.15).

The right-hand sides of (3.14), (3.15), (3.22), and (3.23), (3.28), (3.29), (3.33), and (3.34) are finite; and, provided that the expressions used in the investigation of neighborhoods of conjugate points involve only the proper combinations of vanishing eigenvalues and vanishing determinants, we are now equipped to compute probability amplitudes for transitions between conjugate points.

C. Probability amplitudes in the Airy regime (Ref. 17)

In this section, we consider position-to-position, momentum-to-position, and position-to-momentum transitions; momentum-to-momentum transitions are computed in Sec. IV. We consider a system whose Lagrangian is $L(q,\dot{q})=\frac{1}{2}|\dot{q}|^2-V(q)$ and transitions between conjugate points which have multiplicity 1, i.e., the Jacobi operators are assumed to have only one zero eigenvalue: $\alpha^1=0$.

(i) Position-to-position transitions (Ref. 18, and see Fig. 2).

We compute $\mathscr{K}(b^\Delta,t_b;a,t_a)$, given by (A45) with the initial wave function given by (A50), for b^Δ close to the caustic on the bright or dark side. We shall show that, although the limit of $\mathscr{K}_{\rm WKB}(b^\Delta,t_b;a,t_a)$ when b^Δ tends to a conjugate point b is infinite, the limit of $\mathscr{K}(b^\Delta,t_b;a,t_a)$ is well defined. We shall not compute $\mathscr{K}$ by expanding around the classical path(s) defined by (a,t_a) and (b^Δ,t_b) for the following reasons.

If b^Δ is on the dark side of the caustic, there is no classical path defined by the given boundary values $(a,t_a),(b^\Delta,t_b)$. If b^Δ is on the bright side of the caustic there may be one or two[19] classical paths defined by the boundary values depending on whether the paths q_1 and q_2, which start at (a,t_a), arrive at b^Δ at the same time or not. Let $\mathscr{K}_1(b^\Delta,t_{(1)b};a,t_a)$ and $\mathscr{K}_2(b^\Delta,t_{(2)b};a,t_a)$ be the semiclassical expansions (WKB and beyond) of $\mathscr{K}$ around q_1 and q_2, respectively. If we try to compute $\mathscr{K}$ as the sum of two contributions

$$\mathscr{K}(b,t_b;a,t_a)=\lim_{\substack{b^\Delta\to b\\ t_{(i)b}\to t_b}}\left(\mathscr{K}_1(b^\Delta,t_{(1)b};a,t_a)+\mathscr{K}_2(b^\Delta,t_{(2)b};a,t_a)\right)\ ,$$

we are faced with a delicate situation: when b^Δ tends to b the WKB approximations of $\mathscr{K}_1$ and $\mathscr{K}_2$ tends to infinity, and their sum tends also to infinity because one of the path has touched the caustic for $t\in[t_a,t_b]$ and the corresponding amplitude has "picked up" an additional phase equal to $-\pi/2$. One can push the calculation of $\mathscr{K}_1$ and $\mathscr{K}_2$ beyond their WKB approximations, but as q_1 and q_2 coalesce, $\mathscr{K}_1+\mathscr{K}_2$ exhibits some peculiarities whose analysis is subtle. Thus to compute $\mathscr{K}(b^\Delta,t_b;a,t_a)$, we shall proceed via the following steps.

(a) Change the variable of integration in (A45) from $y\in Y_+$ to $f\in Y_+$ defined by

$$b^\Delta+\mu y(t)=q(t)+(b^\Delta-b)(t-t_a)/T+\mu f(t)\ , \tag{3.35}$$

where

$$\mu^2=\hbar/m\ ,\quad T=t_b-t_a\ ,$$

and where q is the unique classical path between the conjugate points (a,t_a) and (b,t_b). The term $(b^\Delta-b)(t-t_a)/T$ is chosen so that

$f\in Y_+$, i.e., $f(t_b)=0$;

the initial wave function (A50) enters

(A45) via $\delta(b^\Delta+\mu y(t_a)-a)=\delta(\mu f(t_a))$,

hence $f(t_a)=0$. (3.36)

This change of variable introduces the following terms[20] in the exponential in the integrand of (A45):

$$\tfrac{1}{2}\mu^{-2}\int_T|\dot{q}(t)+\Delta/T|^2dt-\frac{1}{\mu}\int_T(\ddot{q}(t)\,|\,f(t))dt\ ,\qquad \Delta\equiv b^\Delta-b\ . \tag{3.37}$$

(b) Expanding

$$V\left[q(t)+\Delta\frac{t-t_a}{t_b-t_a}+\mu f(t)\right]$$

in powers of μ up to order 3 gives

$$V(q+\Delta\tau+\mu f)=V(q+\Delta\tau)+\mu(V_{,\alpha}(q)f^{\alpha}+V_{,\alpha\beta}(q)f^{\alpha}\Delta^{\beta}\tau)+\tfrac{1}{2}\mu^2V_{,\alpha\beta}(q+\Delta\tau)f^{\alpha}f^{\beta}$$
$$+\tfrac{1}{6}\mu^3V_{,\alpha\beta\gamma}(q+\Delta\tau)f^{\alpha}f^{\beta}f^{\gamma}+\cdots\ . \tag{3.38}$$

The gradient of V has been expanded around q so that one can see at a glance how the equation of motion $m\ddot{q}_{\alpha}+V_{,\alpha}(q)=0$ simplifies the sum of (3.37) and

$$-(\mu^2m)^{-1}V\left[q(t)+\Delta\frac{t-t_a}{t_b-t_a}+\mu f(t)\right]$$

needed in the calculation of $\mathscr{K}(b^{\Delta},t_b;a,t_a)$

(c) Change the integration over Y_+ with respect to the integrator w_+^w into an integration over the space Y of paths f vanishing at t_a and t_b, carried on with respect to a new integrator w^w.

(d) Use the Cameron-Martin transformation to express the integral in terms of an integrator w which "absorbs" the bilinear terms in f, namely

$$V_{,\alpha\beta}(q(t)+\Delta(t-t_a)/T)f^{\alpha}(t)f^{\beta}(t)\ .$$

However, the formulas developed in Ref. 1 for this purpose are valid when the argument of $V_{,\alpha\beta}$ is a classical path q and when $q(t_a)$ and $q(t_b)$ are not conjugate. But here the argument of $V_{,\alpha\beta}$, namely $q(t)+\Delta(t-t_a)T^{-1}$, is not a classical path; its limit when Δ tends to zero *is* a classical path, but one whose end points are conjugate. Thus we shall have to replace q by a classical path $\bar{q}$ very close to q in order to carry on the Cameron-Martin transformation that absorbs $V_{,\alpha\beta}[\bar{q}(t)]f^{\alpha}(t)f^{\beta}(t)$. We shall take the limit of $\bar{q}$ tending to q after step *e*. The result can be read off of similar results carried out in full detail in Ref. 1 [e.g., (3.28) in 1]:

$$\mathscr{K}(b^{\Delta},t_b;a,t_a)=\exp\left[\frac{i}{\hbar}\underline{S}(\underline{q}^{\Delta},t_b,t_a)\right]\bar{I} \tag{3.39}$$

with

$$\bar{I}\equiv(2\pi i\hbar)^{-n/2}\left|\det_{\alpha\beta}\bar{J}^{\alpha\beta}(t_b,t_a)\right|^{-1/2}\int_Y d\bar{w}(f)$$
$$\times\exp\left[-\frac{i}{\hbar}\int_T\left[V_{,\alpha\beta}(q(t))f^{\alpha}(t)\Delta^{\beta}(t-t_a)T^{-1}+\frac{\mu^3}{6}V_{,\alpha\beta\gamma}(q(t))f^{\alpha}(t)f^{\beta}(t)f^{\gamma}(t)+O(\mu^2)+O(\Delta)\right]dt\right]\ , \tag{3.40}$$

where the barred quantities are computed in terms of $\bar{q}$ and where $\underline{S}(\underline{q}^{\Delta},t_b,t_a)$ is the action functional computed along

$$q^{\Delta}(t)\equiv q(t)+\Delta(t-t_a)T^{-1}\ .$$

Note that $\underline{S}$ computed for q^{Δ} is not an action function because q^{Δ} is not a classical path.

(e) The path integral (3.40) can be computed by making a change of variable of integration from $\mu f\in Y$ to $\bar{u}\in\mathbb{R}^n$ which diagonalizes the variance of the integrator $\bar{w}$. Let $\bar{\psi}_k^{\mu}(t)$ be the eigenfunctions of the Jacobi operator $\mathscr{F}(\bar{q})$ with Dirichlet boundary conditions (3.5). Let

$$\mu f^{\mu}(t)=\sum_{k=1}^{\infty}\bar{u}^k\bar{\psi}_k^{\mu}(t)\ ,\quad \bar{\psi}(t_a)=0\ ,\quad \bar{\psi}(t_b)=0\ , \tag{3.41}$$

and let P be the projection

$$P:\ Y\to\mathbb{R}^n\ \text{by}\ f\to\bar{u}\equiv\{\bar{u}^1,\bar{u}^2,\dots\}\ ; \tag{3.42}$$

then the image $P\bar{w}$ of $\bar{w}$ under P is the Gaussian (see Ref. 1, p. 316)

$$d(P\bar{w})(\bar{u})=\exp\left[-\frac{i}{2\mu^2}\sum_{k=1}^{\infty}\bar{\alpha}_k(\bar{u}^k)^2\right]\prod_{k=1}^{\infty}(-\bar{\alpha}_k/2\pi i\mu^2)^{1/2}d\bar{u}^k\ . \tag{3.43}$$

By virtue of (3.14) the limit I of $\bar{I}$ when $\bar{q}$ tends to q is

$$I=(2\pi i\hbar)^{-n/2}(-2\pi i\hbar)^{-1/2}\left[\det_{\alpha\beta}\hat{J}^{\alpha\beta}(t_b,t_a)/\dot{\psi}_{(1)}^2(t_a)\dot{\psi}_{(1)2}(t_b)\right]^{-1/2}$$
$$\times\int_{\mathbb{R}^n}\prod_{k=2}^{\infty}(-\alpha_k/2\pi i\hbar)^{1/2}du^1du^2\cdots\exp\left[-\frac{i}{2\mu^2}\sum_{k=2}^{\infty}\alpha_k(u^k)^2\right.$$
$$\left.-\frac{i}{m\mu^2}\sum_{k=1}^{\infty}[\mathscr{V}_{k\beta}\Delta^{\beta}u^k+\tfrac{1}{6}\mathscr{V}_{jkl}u^ju^ku^l+O(\Delta)+O(\mu^2)]\right]\ , \tag{3.44}$$

where

$$\mathscr{V}_{k\beta}\Delta^{\beta} \equiv \int V_{,\alpha\beta}(q(t))\psi_k^{\alpha}(t)\Delta^{\beta}(t-t_a)T^{-1}dt \; ,$$

$$\mathscr{V}_{jkl} \equiv \int V_{,\alpha\beta\gamma}(q(t))\psi_j^{\alpha}(t)\psi_k^{\beta}(t)\psi_l^{\gamma}(t)dt \; .$$

In Ref. 1 we used erroneously $\alpha_1{}^{-1}\det J(t_b,t_a) = \det\hat{J}(t_b,t_a)$, which is valid only in special cases, whereas (3.14) is valid in all cases. Integrating over $u^2, u^3 \ldots$ and keeping only the terms of lowest order in Δ and in μ one obtains

$$I = (2\pi i\hbar)^{-n/2}(-2\pi i\hbar)^{-1/2}\left|\det_{\alpha\beta}\hat{J}^{\alpha\beta}(t_b,t_a)/\dot{\psi}^1_{(1)}(t_a)\dot{\psi}_{(1)1}(t_b)\right|^{-1/2} I(\nu,c) \; , \tag{3.45}$$

where $I(\nu,c)$ is the integral over u^1,

$$I(\nu,c) = \int_R du \exp\left[i\left[cu - \frac{\nu}{3}u^3\right]\right] , \tag{3.46}$$

where

$$\nu = \frac{1}{2\hbar}\mathscr{V}_{111}$$

and

$$c = -\frac{1}{\hbar}\mathscr{V}_{1\beta}\Delta^{\beta}$$

with $\mathscr{V}_{111}$ and $\mathscr{V}_{1\beta}$ defined as in Eq. (3.44). $I(\nu,c)$ is the Airy function of argument $\nu^{-1/3}c$ normalized to $\nu^{-1/3}$:

$$I(\nu,c) = \nu^{-1/3}\int_R dv \exp[i(\nu^{-1/3}cv - \tfrac{1}{3}v^3)]$$

$$\equiv \nu^{-1/3}\mathrm{Ai}(\nu^{-1/3}c) \; . \tag{3.47a}$$

We now compute the normalizing factor ν of the Airy function and its argument $\nu^{-1/3}c$. To compute c we note that the Jacobi field ψ_1 satisfies

$$-\ddot{\psi}^{\alpha}_{(1)} - \nabla^{\alpha}\nabla_{\beta}V(q(t))\psi^{\beta}_{(1)} = 0 \; ,$$

hence

$$\begin{aligned} c &= -\frac{1}{\hbar}\mathscr{V}_{1\beta}\Delta^{\beta} \\ &= -\frac{1}{\hbar}\int V_{,\alpha\beta}(q(t))\psi_1^{\alpha}(t)\Delta^{\beta}(t-t_a)T^{-1}dt \\ &= \frac{\Delta^{\beta}}{\hbar T}\int_T \ddot{\psi}_{1\beta}(t-t_a)dt \\ &= \frac{\Delta^{\beta}}{\hbar T}\left[(t-t_a)\dot{\psi}_{1\beta}\Big|_{t_a}^{t_b} - \int_{t_a}^{t_b}\dot{\psi}_{1\beta}dt\right] \\ &= \frac{1}{\hbar}(b^{\Delta} - b \mid \dot{\psi}_1(t_b)) \; . \end{aligned} \tag{3.47b}$$

The computation of ν is an exercise in solving the small disturbances of the small disturbance equation (i.e., the small disturbances of the Jacobi equation) with the appropriate Green's function of the small disturbance equation. Let $\{q(\alpha)\}_{\alpha}$ be a one-parameter family of classical paths such that

$q(\alpha_0)$ is the path defined by $(a,t_a),(b,t_b)$;

$\partial q(\alpha)/\partial\alpha\,|_{\alpha_0} = \psi_1$ is the Jacobi field vanishing at t_a and t_b,

$q(t_a,\alpha) = a$ for all α and

$$\dot{q}(t_a,\alpha) = \alpha\dot{\psi}_1(t_a) = \alpha\,\partial\dot{q}(t_a,\alpha_0)/\partial\alpha_0 \; ,$$

i.e.,

$$\partial^2 q(t_a,\alpha)/\partial\alpha^2 = 0 \text{ and } \partial^2\dot{q}(t_a,\alpha)/\partial\alpha^2 = 0 \; .$$

We write $q(t,\alpha)$ instead of $q(\alpha)(t)$ whenever it makes the equation easier to read. For[21] $L(q,\dot{q}) = \frac{1}{2}m^2\|\dot{q}\|^2 - V(q)$, the Jacobi field $\partial q(\alpha)/\partial\alpha$ satisfies

$$\begin{aligned} \left[\mathscr{F}_t(q(\alpha))\left[\frac{\partial q(t,\alpha)}{\partial\alpha}\right]\right]^{\mu} &\equiv \mathscr{F}_t\frac{\partial q^{\mu}}{\partial\alpha}(t,\alpha) \\ &= -\nabla_t{}^2\frac{\partial q^{\mu}}{\partial\alpha}(t,\alpha) \\ &\quad - \nabla^{\mu}\nabla_{\nu}V(q(t,\alpha))\frac{\partial q^{\nu}}{\partial\alpha}(t,\alpha) = 0 \; . \end{aligned} \tag{3.48}$$

Taking the derivative of this equation with respect to α, we obtain the small disturbances of the small disturbance equation:

$$\mathscr{F}_t\frac{\partial^2 q^{\mu}}{\partial\alpha^2}(t,\alpha) = \nabla^{\mu}\nabla_{\nu}\nabla_{\rho}V(q(t,\alpha))\frac{\partial q^{\nu}}{\partial\alpha}\frac{\partial q^{\rho}}{\partial\alpha} \; , \tag{3.49}$$

which can be solved with the Green's function G of $\mathscr{F}_t$ having the same boundary conditions as $\partial^2 q/\partial\alpha^2$, namely the c conditions above:

$$G(t,s) = -\theta(t-s)J(t,s) \; . \tag{3.50}$$

Thus

$$\frac{\partial^2 q^{\mu}}{\partial\alpha^2}(t,\alpha) = -\int_{t_a}^{t} ds J^{\mu\sigma}(t,s)\nabla_{\sigma}\nabla_{\nu}\nabla_{\rho}V(q(s,\alpha)) \times\frac{\partial q^{\nu}}{\partial\alpha}(s)\frac{\partial q^{\rho}}{\partial\alpha}(s) \; .$$

Setting $t = t_b$ and $\alpha = \alpha_0$, taking the scalar product of both sides with $\partial\dot{q}(t_b,\alpha_0)/\partial\alpha_0$, and using Eq. (3.11),

$$-[\partial\dot{q}_{\mu}(t_b,\alpha_0)/\partial\alpha_0]J^{\mu\sigma}(t_b,s) = \partial q^{\sigma}(s,\alpha_0)/\partial\alpha_0 \; ,$$

one obtains

$$\begin{aligned} \nu &= -\frac{1}{2\hbar}\left[\frac{\partial\dot{q}}{\partial\alpha_0}t_b,\alpha_0)\Big|\frac{\partial^2 q}{\partial\alpha_0{}^2}(t_b,\alpha_0)\right] \\ &= -\frac{1}{2\hbar}\int_{t_a}^{t_b}\nabla_{\sigma}\nabla_{\nu}\nabla_{\rho}V(q(t,\alpha_0))\frac{\partial q^{\sigma}}{\partial\alpha_0}\frac{\partial q^{\nu}}{\partial\alpha_0}\frac{\partial q^{0}}{\partial\alpha_0}dt \; . \end{aligned} \tag{3.51}$$

Of course, a similar calculation with an α family of paths with zero boundary conditions at t_b would have given the scaling factor ν in terms of the derivatives at t_a. The point here is that ν given as an integral over the third derivative of the potential is now given in terms of the Jacobi field ψ_1 at one end point and the variation of the Jacobi fields at ψ_1.

When $\hbar$ tends to zero, the leading contribution of the Airy function is for the value u_0 of u which makes the phase $\nu^{-1/3}cv - \frac{1}{3}v^3$ stationary, i.e., $v_0{}^2 = \nu^{-1/3}c$. Note that v_0 is of order $\hbar^{-1/3}$. For $\hbar$ vanishingly small,

$$\mathrm{Ai}(\nu^{-1/3}c) \simeq \begin{cases} 2\sqrt{\pi}v_0{}^{-1/4}\cos\left[\frac{2}{3}v_0{}^3 - \frac{\pi}{4}\right], & v_0 > 0\,, \\ \sqrt{\pi}(-v_0)^{-1/4}\exp\left[-\frac{2}{3}v_0{}^3\right], & v_0 < 0\,. \end{cases}$$

For $u_0 > 0$, b^Δ is in the illuminated region and the probability amplitude oscillates rapidly. For $u_0 < 0$, b is in the shadow region and the probability amplitude decays exponentially. Since $u_0{}^3 = \nu c^{3/2}$ is proportional to $(m/\hbar)\,|\,b^\Delta - b\,|^{3/2}$, quantum mechanics can be said to "soften up" the caustics. The probability amplitude $\mathscr{K}(b^\Delta,t_b;a,t_a)$ does not blow up when b^Δ tends to b. It is valid on and near the caustic, in the dark, and in the bright region for $|\,b^\Delta - b\,| \sim \hbar/mc$.

(ii) Momentum-to-position transitions (see Fig. 3).

Since we want to apply this study to scattering problems, we shall compute the momentum-to-position probability amplitude $\mathscr{K}(b,t_b;p_a,t_a)$ for t_a equal to $-\infty$ and p_a equal to an initial momentum p_i. We assume b to be on the caustic formed by the family of classical paths with initial momentum p_i and b^Δ close to b. We compute

$$\mathscr{K}(b^\Delta,t_b;p_i,-\infty) = W_+(b^\Delta,p_i)\exp\left[\frac{i}{\hbar}\langle p_i,b^\Delta\rangle\right], \tag{3.52}$$

where $W_+(x,p_i)$ is the Møller wave operator given by the path integral (see Ref. 1, pp. 292—293, 366—367)

$$W_+(b^\Delta,p_i) = \int_{Y_+} dw_+^W(y)\exp\left[-\frac{i}{\mu^2}\int_{-\infty}^{t_b}\frac{1}{m}V(b^\Delta + p_i(t-t_b)/m + \mu y(t))dt\right], \quad \mu^2 \equiv \hbar/m\,, \tag{3.53}$$

where w_+^W is the normalized Gaussian on the space of continuous paths $y \in Y_+$ such that $y(t_b) = 0$. Its covariance is

$$G_+^W(t,s) = \theta(s-t)(t_b - s)\mathbb{1} + \theta(t-s)(t_b - t)\mathbb{1}\,.$$

The calculation of $w_+(b^\Delta,p_i)$ proceeds via the following steps.

(a) Change the variable of integration in (3.53) from $y \in Y_+$ to $f \in Y_+$ defined by

$$b^\Delta + p_i(t-t_b)/m + \mu y(t) = q(t) + b^\Delta - b + \mu f(t)\,, \tag{3.54}$$

where q is the unique classical path defined by the boundary conditions $(p_i,-\infty)$ and (b,t_b) and where the added term $\Delta \equiv b^\Delta - b$ is such that

$$f(t_b) = 0 \text{ and } \dot{f}(-\infty) = 0\,. \tag{3.55}$$

This change of variable introduces the following terms in the exponential of (3.53):

$$\int_{-\infty}^{t_b} dt\left[\frac{1}{2\mu^2}\,||\dot{q}(t) - p_i/m\,||^2 - \frac{1}{\mu}(\ddot{q}(t)\,|\,f(t))\right]. \tag{3.56}$$

(b) Expand $V(q + \Delta + \mu f)$ in powers of μ up to order 3.

(c) Use the Cameron-Martin transformation to express the integral in terms of an integrator $\bar{w}_+$ which absorbs the bilinear term in f. Here again we have to replace q by a classical path $\bar{q}$ very close to q, carry on the Cameron-Martin transformation that absorbs $V_{,\alpha\beta}[\bar{q}(t)]f^\alpha(t)f^\beta(t)$, then take the limit when $\bar{q}$ tends to q.

(d) Compute the path integral by making a change of variable of integration from $f \in Y$ to $\bar{u} \in \mathrm{R}^n$ which diagonalizes the variance of the integrator $\bar{w}_+$. Let $\bar{\psi}_k(t)$ be the eigenfunctions of the Jacobi operator $\mathscr{T}(\bar{q})$ with mixed boundary conditions of type b. Let f be expanded in terms of these eigenfunctions as in (3.41) and P be defined as in (3.42). By virtue of (3.22), we obtain a result similar to (3.44). Integrating over $u^2, u^3, \ldots$ and keeping only the terms of higher order in Δ and in μ, one obtains

$$W_+(b^\Delta,p_i) = \exp\left[\frac{i}{\hbar}\int_{-\infty}^{t_b}\left[\tfrac{1}{2}\,|\,\dot{q}(t) - p_i/m\,|^2 - V(q(t)+\Delta)\right]dt\right] I\,, \tag{3.57}$$

$$I = (-2\pi i\hbar)^{-1/2}\left[\det_{\alpha\beta}\hat{K}^{\alpha\beta}(t_b,t_a)/\psi^1_{(1)}(-\infty)\dot{\psi}_{(1)1}(t_b)\right]^{-1/2} I(\nu,c)\,, \tag{3.58}$$

and where $I(\nu,c)$ is the Airy function (3.46) with $\mathscr{V}_{1\beta}$ and $\mathscr{V}_{111}$ given in terms of the Jacobi eigenfunctions $\psi_k^\mu(t)$ with mixed boundary conditions $\dot{\psi}(-\infty) = 0$, $\psi(t_b) = 0$ by

$$\mathscr{V}_{1\beta} \equiv \int V_{,\alpha\beta}(q(t))\psi_1^\alpha(t)dt\,,$$

$$\mathscr{V}_{111} \equiv \int V_{,\alpha\beta\gamma}(q(t))\psi_1^\alpha(t)\psi_1^\beta(t)\psi_1^\gamma(t)dt\,,$$

Equations (3.57) and (3.58) give the Møller wave operator $W_+(b^\Delta,p_i)$ for $b^\Delta = b + \Delta$ on or near the caustic, on the dark or on the bright side.

We shall now discuss the Airy regime of $W_+(b^\Delta, p_i)$.

The normalizing factor ν of the Airy function is given by the same expression as the normalizing factor for the position-to-position amplitude, but in terms of a different Jacobi field. To compute it we introduce the α family $\{q(\alpha)\}$ of classical paths such that

$q(\alpha_0)$ is the path defined by the boundary conditions and

$$(p_i, -\infty);(b,t_b) ;$$

$\partial q(\alpha)/\partial\alpha\,|_{\alpha_0}=\psi_1$ is the Jacobi field with

mixed boundary conditions ;

$m\dot{q}(-\infty,\alpha)=p_i$ for all α; and

$$q(-\infty,\alpha)=\alpha\,\partial q(-\infty,\alpha_0)/\partial\alpha_0 \text{ , i.e. ,}$$

$$\partial^2 q(-\infty,\alpha)/\partial\alpha^2=0 \text{ and } \partial^2\dot{q}(-\infty,\alpha)/\partial\alpha^2=0 \ . \tag{3.59}$$

A calculation similar to the one in Sec. III C (i), but using (3.18) instead of (3.11), gives

$$\nu=-\frac{1}{2\hbar}\left[\frac{\partial\dot{q}}{\partial\alpha_0}(t_b,\alpha_0)\,\middle|\,\frac{\partial^2 q}{\partial{\alpha_0}^2}(t_b,\alpha_0)\right] , \tag{3.60}$$

i.e., the same expression as before but for a different α family; and

$$\begin{aligned} c=-\frac{1}{\hbar}\mathscr{V}_{1\beta}\Delta^\beta &= -\frac{\Delta^\beta}{\hbar}\int V_{,\alpha\beta}(q(t))\psi_1^\alpha(t)dt \\ &= \frac{\Delta^\beta}{\hbar}\int \ddot{\psi}_{1\beta}dt=\frac{\Delta^\beta}{\hbar}\dot{\psi}_{1\beta}(t_b) \\ &= \frac{1}{\hbar}(b^\Delta-b\mid\dot{\psi}_1(t_b)) \ , \end{aligned} \tag{3.61}$$

the same expression as (3.47) but for a different α family.

(iii) Position-to-momentum transitions (see Fig. 4).

We shall compute $\mathscr{K}(p_f,\infty;a,t_a)$ when p_f is conjugate to a in the sense that there is one nonzero Jacobi field h along the classical path q defined by $(a,t_a),(p_f,\infty)$, such that

$$h(t_a)=0 \ , \ \ \dot{h}(\infty)=0 \ .$$

We compute first

$$\mathscr{K}(p_f^\Delta,\infty;a,t_a)=W_-^*(a,p_f^\Delta)\exp\left[-\frac{i}{\hbar}(p_f^\Delta,a)\right] , \quad \text{for } p_f^\Delta \text{ close to } p_f \ , \tag{3.62}$$

where $W_-(a,p_f^\Delta)$ is the Møller wave operator (see Ref. 1, pp. 292—293 and 366—367):

$$W_-^*(a,p_f^\Delta)=\int_{Y_-} dw_-^W(y)\exp\left[-\frac{i}{\mu^2}\int_{t_a}^\infty V(a+p_f^\Delta(t-t_a)/m+\mu y(t))dt\right] , \tag{3.63}$$

and w_-^W is the normalized Gaussian on the space of continuous paths $y\in Y_-$ such that

$$G_-^W(t,s)=\theta(s-t)(s-t_a)\mathbb{1}+\theta(t-s)(t-t_a)\mathbb{1} \ . \tag{3.64}$$

The calculation of (3.67) proceeds via the same steps as the calculation of the other Møller operator (3.46):

(a) Change of variable of integration from y to f defined by

$$a+p_f^\Delta(t-t_a)/m+\mu y(t)=q(t)+\Delta(t-t_a)+\mu f(t) \ , \tag{3.65}$$

where $\Delta=(p_f^\Delta-p_f)/m$,

$$y(t_a)=\dot{y}(+\infty)=f(t_a)=\dot{f}(+\infty)=0 \ .$$

This change of variables introduces the following terms in the exponential of the integrand (3.63):

$$\begin{aligned} &\int_{t_a}^{t_b} dt\left[\frac{1}{2\mu^2}||\dot{q}(t)-p_f^\Delta/m||^2+\frac{1}{\mu}\left[\dot{q}(t)-p_f^\Delta/m\,\middle|\,\dot{f}(t)+\frac{\Delta}{\mu}\right]+\left[\frac{\Delta}{\mu}\,\middle|\,\dot{f}(t)\right]+\frac{1}{2\mu^2}\Delta^2\right] \\ &\qquad =\int_{t_a}^{t_b} dt\left[\frac{1}{2\mu^2}||\dot{q}(t)-p_f^\Delta/m||^2+\frac{1}{2\mu^2}\Delta^2+\frac{1}{\mu^2}(\dot{q}(t)-p_f^\Delta/m\mid\Delta)-\frac{1}{\mu}(\ddot{q}(t)\,|\,f(t))\right] . \end{aligned} \tag{3.66}$$

(b) Expand V around $V(q^\Delta)$, where $q^\Delta=q(t)+\mu\Delta(t-t_a)$,

$$\begin{aligned} V(q^\Delta(t)+\mu f(t)) &= V(q^\Delta)+\mu\nabla_\mu V(q^\Delta)f^\mu(t)+\frac{\mu^2}{2}\nabla_\mu\nabla_\nu V(q^\Delta)f^\mu(t)f^\nu(t) \\ &\quad +\frac{\mu^3}{6}\nabla_\mu\nabla_\nu\nabla_\rho V(q^\Delta)f^\mu(t)f^\nu(t)f^\rho(t)+O(\mu^4) \\ &= V(q^\Delta)+\mu\nabla_\mu V(q)f^\mu(t)+\mu^2\nabla_\nu\nabla_\mu V(q)f^\mu(t)\cdot\Delta^{\nu}\cdot(t-t_a)+\frac{\mu^2}{2}\nabla_\mu\nabla_\nu V(q)f^\mu(t)f^\nu(t) \\ &\quad +\frac{\mu^3}{6}\nabla_\mu\nabla_\nu\nabla_\rho V(q)f^\mu(t)f^\nu(t)f^\rho(t)+O(\mu^4)+O(\mu^3\Delta) \ . \end{aligned} \tag{3.67}$$

Combining this expansion with the terms introduced by the change of variable gives

$$W^*_-(a,p_f^\Delta)=\exp\left[\frac{i}{\hbar}\int_{t_a}^{\infty}\left[\frac{m}{2}\mid \dot q(t)-p_f/m\mid^2-V(q(t)+\Delta(t-t_a))\right]dt\right]I\ . \tag{3.68}$$

Similarly, as the cases (a) and (b), we obtain

$$I=(-2\pi i\hbar)^{-1/2}[\det_{\mu\nu}\hat{\tilde K}_\mu{}^\nu(t_b,t_a)/\dot\psi^1_{(1)}(t_a)\psi^1_{(1)}(\infty)]^{-1/2}I(\nu,c)\ , \tag{3.69}$$

where $I(\nu,c)$ is the Airy function (3.46) with $\mathscr{V}_{1\beta}$ and $\mathscr{V}_{111}$ given in terms of the Jacobi eigenfunction $\psi^\mu_k(t)$ with mixed boundary conditions $\psi(t_a)=0$ and $\dot\psi(\infty)=0$ by

$$\begin{aligned}\mathscr{V}_{1\beta}&=\int_{t_a}^{\infty}V_{,\alpha\beta}(q(t))(t-t_a)\psi_1^\alpha(t)dt\ ,\\ \mathscr{V}_{111}&=\int_{t_a}^{\infty}V_{,\alpha\beta\gamma}(q(t))\psi_1^\alpha(t)\psi_1^\beta(t)\psi_1^\gamma(t)dt\ .\end{aligned} \tag{3.70}$$

Equations (3.68) and (3.69) give the Møller wave operator $W^*_-(a,p_f^\Delta)$ for $p_f^\Delta=p_f+\Delta$ on or near the caustic, on the dark or on the bright side. To compute the factor ν of the Airy function, we introduce the α family $\{q(\alpha)\}$ of classical paths such that

$q(\alpha_0)$ is the path defined

by (a,t_a), (p_f,∞) ,

$\partial q(\alpha)/\partial\alpha\mid_{\alpha_0}=\psi_1$ is the Jacobi field with

mixed boundary conditions ,

$q(t_a,\alpha)=a$ for all α and

$$\dot q(t_a,\alpha)=\alpha\dot\psi_1(t_a)=\alpha\frac{\partial\dot q(t_a,\alpha_0)}{\partial\alpha_0},$$

i.e. ,

$$\frac{\partial^2q(t_a,\alpha)}{\partial\alpha^2}=0 \text{ and } \frac{\partial^2\dot q(t_a,\alpha)}{\partial\alpha^2}=0\ . \tag{3.71}$$

A calculation similar to (a) and (b) gives

$$\nu=-\frac{1}{2\hbar}\left[\frac{\partial^2\dot q}{\partial\alpha_0{}^2}(\infty,\alpha_0)\middle|\frac{\partial q}{\partial\alpha_0}(\infty,\alpha_0)\right] \tag{3.72}$$

and

$$\begin{aligned}c&=-\frac{1}{\hbar}\mathscr{V}_{1\beta}\Delta^\beta\\ &=-\frac{1}{\hbar}\Delta^\beta\int_{t_a}^{\alpha}V_{,\alpha\beta}(q(t))(t-t_a)\psi_1^\alpha(t)dt\\ &=-\frac{1}{\hbar}(p_f^\Delta-p_f/m\mid\psi_1(\infty))\ .\end{aligned} \tag{3.73}$$

IV. PATH INTEGRAL REPRESENTATION OF THE S MATRIX

A. Introduction

The reason one cannot construct a Feynman-Kac formula for momentum-to-momentum transitions similar to the ones for position-to-position and momentum-to-position ones is the fact that there is no Green's function of $-d^2/dt^2$ whose derivatives vanish at both end points, and hence there is no Gaussian integrator for the free particle. However a Feynman-Kac formula for scattering theory has recently been constructed from two different approaches. In the first approach,[12] one constructs it from a phase-space Feynman-Kac path integral whose covariance is the Green's function of the Jacobi operator with vanishing derivatives at both end points. The second approach[13] to scattering theory begins with the scattering wave function $\psi(x,t)$ for an initial state of a plane wave. This wave function is equivalent to the transition amplitude we have called $K(b,t_b;p_a,t_a)$. The advantage of this approach is that the path integral for $K(b,p_a)$ is well developed.[1] The ostensible disadvantage is that the caustics in scattering theory are momentum-to-momentum caustics, not momentum-to-positions ones. However, these two types of caustics can be related in the scattering limit of $t_b\to\infty$ and $t_a\to-\infty$. In particular, in this limit, the integrators for the semiclassical expansions of $K(p_b;p_a)$ and $K(b;p_a)$ and their normalizations are equal. Both approaches lead to the same Feynman-Kac formula for scattering theory. This formula has two advantages: In the present context it gives directly quantitative answers to the caustic problem which have an easy intuitive interpretation, and it provides a unified treatment of all four cases. In general, it allows us to use directly all of the elegance and power of the well-developed theory of prodistributions for path integrals.[1]

Another difficulty presented by momentum-to-momentum transitions which has also been solved recently[2] is the existence of constraints between the initial and final momenta due to conservation laws, and we summarize in the following section the results obtained in Ref. 2.

B. The WKB approximations

(i) Transitions during a finite time interval.

In the previous paper,[2] we considered momentum-to-momentum amplitudes $\mathscr{K}(\phi_b,t_b;\phi_a,t_a)$ when t_a and t_b are very large but not infinite, for a system with Lagrangian $L=\frac{1}{2}||\dot q||^2-V(q)$. We have computed[22]

$$\mathscr{K}_{\rm WKB}(\phi_b,t_b;\phi_a,t_a)\equiv\lim_{\hbar\to0}\int_M dx\,\mathscr{K}_{\rm WKB}(\phi_b,t_b;x,t)\mathscr{K}_{\rm WKB}(x,t;\phi_a,t_a)\ , \tag{4.1}$$

where $\mathscr{K}_{\rm WKB}(x,t;\phi_a,t_a)$ is the WKB approximation of $\psi_a(x,t)$ given by (A.45) for the initial value $\phi_a(\cdot)=T_a(\cdot)\exp i/\hbar S_a(\cdot)$ and $\mathscr{K}_{\rm WKB}(\phi_b,t_b;x,t)$ is the WKB approximation of $\phi_b(x,t)$ given by (A46) for ϕ_b defined similarly to ϕ_a. These WKB approximations are easily expressed in terms of the classical flows Φ and Ψ on M corresponding to the initial and final wave functions ϕ_a and ϕ_b. Namely, let Φ_s: $M \to M$ be the classical flow defined by

$$\ddot{\Phi}_s(a) = -\nabla V(\Phi_s(a)) \text{ with } \ddot{\Phi}_s = d^2\Phi_s/ds^2,\ a \in M \tag{4.2a}$$

$$\Phi_0(a) = a,\quad \dot{\Phi}_0(a) = \nabla S_a(a)\ . \tag{4.2b}$$

Then the classical path defined by the boundary values (ϕ_a, t_a) and (x,t) is

$$\Phi_{s-t_a} \circ \Phi_{t-t_a}{}^{-1}(x)\ . \tag{4.3}$$

Let Ψ_s: $M \to M$ be the classical flow defined by

$$\ddot{\Psi}_s(a) = -\nabla V(\Psi_s(a))\ , \tag{4.4a}$$

$$\Psi_0(a) = a,\quad \dot{\Psi}_0(a) = \nabla S_b(a)\ ; \tag{4.4b}$$

then the classical path defined by $(s,t),(\phi_b,t_b)$ is

$$\Psi_{s-t_b} \circ \Psi_{t-t_b}{}^{-1}(x)\ . \tag{4.5}$$

If there is no path belonging to both flows, and if T_a and T_b are of compact support, the $\mathscr{K}_{\text{WKB}}(\phi_b,t_b;\phi_a,t_a)$ defined by (4.1) is of order $\hbar^n$, with n an arbitrary integer. If there is one, and only one classical path defined by $(\phi_a,t_a),(\phi_b,t_b)$, then

$$\mathscr{K}_{\text{WKB}}(\phi_b,t_b;\phi_a,t_a) = (2\pi\hbar)^l \delta(c_1)\delta(c_2)\cdots\delta(c_l)\hat{\mathscr{K}}_{\text{WKB}}(\phi_b,t_b;\phi_a,t_a)\ , \tag{4.6}$$

where $\{c_i = 0:\ i = 1, \ldots, l\}$ are the l conservation laws that ∇S_a and ∇S_b must satisfy if there is to be a classical path belonging to both flows. The quantity $\hat{\mathscr{K}}_{\text{WKB}}(\phi_b,t_b;\phi_a,t_a)$, whose square determines the cross section, is equal to

$$\hat{\mathscr{K}}_{\text{WKB}}(\phi_b,t_b;\phi_a,t_a) = (2\pi\hbar)^{(n-l)/2}\exp[(q-p)i\pi/4]\exp\left[\frac{i}{\hbar}S(\phi_b,t_b;\phi_a,t_a)\right]\left[\prod_{A=l+1}^{n}\lambda_A\right]^{-1/2} T_a(q(t_a))T_b(q(t_b)) \tag{4.7}$$

where $S(\phi_b,t_b;\phi_a,t_a)$ is the action function[23] computed for the classical path q belonging to both flows, $\{\lambda_A; A = l+1, \ldots n\}$ are the nonzero eigenvalues of

$$L_{\alpha\beta}(t_b,t_a) = \partial p_\alpha(t_b,a,p_a)/\partial a^\beta$$

taken at $a = q(t_a); q + p = n - l$, and p is the Morse index. When there are no conservation laws imposing constraints on the initial and final momenta, the matrix $L(t_b,t_a)$ is the inverse of the Van Vleck matrix P:

$$P^{\alpha\beta}(t_a,t_b) = \partial^2 S(p_b,t_b;p_a,t_a)/\partial p_a^\alpha \partial p_b^\beta\ .$$

[See Ref. 2, Appendix A, Sec. III, (A15c) and (A37).]

(ii) Transitions during an infinite time interval.

When $t_a = -\infty$ and/or $t_b = \infty$, (4.7) is meaningless. To compute $\mathscr{K}_{\text{WKB}}(p_f,\infty;p_i,-\infty)$, we shall use the beautiful limiting procedure provided by the Møller wave operators (3.53) and (3.63) for systems which approach integrable systems asymptotically[24]; namely,

$$\mathscr{K}(p_f,\infty;p_i,-\infty) = \int_{\mathbb{R}^n} dx\, \mathscr{K}(p_f,\infty;x,t)\mathscr{K}(x,t;p_i,-\infty)$$

for $\mathscr{K}(p_f,\infty;x,t)$ and $\mathscr{K}(x,t;p_i,-\infty)$ given by (3.52) and (3.62), respectively. We assume in this paragraph that $(p_i,-\infty),(x,t)$ defines a unique path q_{in} and that $(x,t),(p_f,\infty)$ defines a unique path q_{fin}. Moreover, we assume (x,t) is not conjugate to $(p_i,-\infty)$ or to (p_f,∞).

The calculation of $\mathscr{K}_{\text{WKB}}(p_f,\infty,x,t)$ and $\mathscr{K}_{\text{WKB}}(x,t;p_i,-\infty)$ is a simplified version of the calculation carried out in Secs. III C (ii) and III C (iii), respectively, namely by

(a) making the change of variable of integration

$$x + p_i(s-t)/m + \mu y(s) = q(s) + \mu f(s)\ ;$$

(b) expanding the potential $V(q+\mu f)$ in powers of μ up to order 2;

(c) making a Cameron-Martin transformation to absorb the terms quadratic in f, one obtains

$$\begin{aligned} I \equiv\ & \mathscr{K}_{\text{WKB}}(p_f,\infty;p_i,-\infty) \\ =\ & \lim_{\hbar\to 0}\int_{\mathbb{R}^n} dx[\det_{\alpha\beta}\tilde{K}_\alpha{}^\beta(\infty,t)\det_{\alpha\beta}K^\alpha{}_\beta(t,-\infty)]^{-1/2} \\ & \times\exp\left\{\frac{i}{\hbar}\int_{-\infty}^{t}\left[\frac{m}{2}||\dot{q}_{\text{in}}(s)-p_i/m||^2 - V(q_{\text{in}}(s))\right]ds\right. \\ & \left. + \frac{i}{\hbar}p_i x + \frac{i}{\hbar}\int_t^{+\infty}\left[\frac{m}{2}||\dot{q}_{\text{fin}}(s)-p_f/m\,||^2 - V(q_{\text{fin}}(s))\right]ds - \frac{i}{\hbar}p_f x\right\}\ . \end{aligned} \tag{4.8}$$

This integral is of the type computed in Ref. 2,

$$I = \lim_{\hbar\to 0}\int_{\mathbb{R}^n} dx \exp\left[\frac{i}{\hbar}F(x)\right]A(x)$$

with $A(x)$ the same determinants as in Ref. 2 and

$$F(x)=\lim_{t_a\to-\infty}\int_{t_a}^{t}\left[\frac{m}{2}||\dot q_{\rm in}(s)||^2-V(q_{\rm in}(s))+\frac{1}{2m}||p_i||^2\right]ds+p_iq_{\rm in}(t_a)$$
$$+\lim_{t_b\to\infty}\int_{t}^{t_b}\left[\frac{m}{2}||\dot q_{\rm fin}(s)||^2-V(q_{\rm fin}(s))+\frac{1}{2m}||p_f||^2\right]ds-p_fq_{\rm fin}(t_b)$$
$$=S(p_f,\infty;x,t)+S(x,t;p_i,-\infty)+\int_{-\infty}^{t}\frac{1}{2m}||p_i||^2ds+\int_{t}^{+\infty}\frac{1}{2m}||p_f||^2ds\ .$$

The dependence of $F(x)$ on x is the same as in Ref. 2. We shall assume in this paragraph that $(p_f,+\infty),(p_i,-\infty)$ defines a unique classical path. The integral (4.8) is then given by an equation similar to (4.6) with

$$\hat{\mathscr{K}}_{\rm WKB}(p_f,\infty;p_i,-\infty)=(2\pi\hbar)^{(n-l)/2}\exp[(q-p)i\pi/4]\exp\left[\frac{i}{\hbar}\left[S(p_f,\infty;p_a,-\infty)+\int_{-\infty}^{+\infty}E\,dt\right]\right]\left[\prod_{A=l+1}^{n}\lambda_A\right]^{-1/2},\tag{4.9}$$

where the notation is the same as in (4.7) and where the term $\delta(|p_i|-|p_f|)$ in (4.6) changes

$$\int_{-\infty}^{t}\frac{1}{2m}||p_i||^2ds+\int_{t}^{\infty}\frac{1}{2m}||p_f||^2ds$$

into $\int_{-\infty}^{+\infty}E\,dt$.

We shall check that the *sum* (and not, as is often claimed, the difference) of the action and the "free" action is a finite phase shift. For q the classical path defined by $(p_i,t_a),(p_f,t_b)$,

$$S(p_f,t_b;p_i,t_a)+\int_{t_a}^{t_b}E\,dt=\int_{t_a}^{t_b}L(q,\dot q)dt+\langle p_i,q(t_a)\rangle-\langle p_f,q(t_b)\rangle+\int_{t_a}^{t_b}E\,dt\tag{4.10}$$
$$=\int_{t_a}^{t_b}\langle p,dq\rangle-\int_{t_a}^{t_b}E\,dt+\langle p_i,q(t_a)\rangle-\langle p_f,q(t_b)\rangle+\int_{t_a}^{t_b}E\,dt\tag{4.11}$$
$$=\int_{t_a}^{t_b}-\langle q,dp\rangle=\int_{t_a}^{t_b}q(t)\nabla V(q(t))dt\ .\tag{4.12}$$

The undefined oscillatory terms

$$\lim_{t_a\to-\infty,t_b\to\infty}\exp\left[-\frac{i}{\hbar}\int_{t_a}^{t_b}E\,dt\right]$$

do not appear in the S-matrix elements $\hat{\mathscr{K}}_{\rm WKB}(p_f,\infty;p_i,-\infty)$. For a potential $V(r)$ decreasing faster than $|r|^{-1}$, the right-hand side of (4.12) remains finite when t_a tends to $-\infty$ and t_b tends to ∞. Coulomb potentials will be discussed in another paper.

C. The Airy regime

In the previous subsection [Eq. (4.9)], we have assumed that in the $(n-l)$-dimensional subspace where $\hat K(p_f,\infty;p_i,-\infty)$ is computed there is one and only one path q defined by $(p_i,-\infty),(p_f,\infty)$. We shall now remove this restriction. That is, we shall assume that there is a nonzero Jacobi field h along q such that

$$\dot h(-\infty)=0,\quad \dot h(\infty)=0\ .\tag{4.13}$$

Again, as in Sec. III C, we shall assume that there is only one such Jacobi field; in other words, the Jacobi operator $\mathscr{J}(q)$ with Neumann boundary conditions has only one zero eigenvalue, say $\alpha^1=0$:

$$\mathscr{J}(q)_{\mu\nu}\psi^{\nu}_{(1)}=0,\quad\text{i.e.,}\quad \psi_{(1)}=h\ .\tag{4.14}$$

We cannot repeat steps (a), (b), (c), (d), and (e) of the three calculations carried on in Sec. III C because we do not have at the present time a Feynman-Kac formula for momentum-to-momentum transitions. However, the form of the three results obtained in Sec. III C, and the results established earlier (the Appendix of Ref. 2, and Sec. III B on the zero eigenvalues of Jacobi operators), dictate a postulate for the fourth one. Moreover, we shall show in Sec. IV D that the rainbow angle obtained with this postulate is equal to the rainbow angle obtained by Ford and Wheeler via the Schrödinger formalism, a fact which considerably strengthens our postulate.

For p_f^{Δ} close to p_f and assuming l conservation laws between the n components of the initial and final momenta,

$$\mathscr{K}(p_f^{\Delta},\infty;p_i,-\infty)=\exp\left[\frac{i}{\hbar}\left[\underline{S}(q^{\Delta},\infty,-\infty)-\langle p_f^{\Delta},q_f^{\Delta}(\infty)\rangle+\langle p_i,q^{\Delta}(-\infty)\rangle+\int_{-\infty}^{+\infty}E\,dt\right]\right]I\ ,\tag{4.15}$$

where the action functional $\underline{S}$ is computed along the path q^{Δ} (not a classical path) given by

$$q^{\Delta}(t)=q(t)+(p^{\Delta}-p)t\ ,$$

where q is the classical path defined by $(p_i,-\infty)$, $(p_f,+\infty)$. I is given by

$$I=(2\pi i\hbar)^{(n-l)/2}\exp[(q-p)^{i\pi/4}(2\pi i\hbar)^{-1/2}]\,|\,\underset{\alpha\beta}{\hat{\det}}L_{\alpha\beta}(\infty,-\infty)/\psi^{1}_{(1)}(-\infty)\psi_{(1)1}(\infty)\,|^{-1/2}I(\nu,c)\ , \tag{4.16}$$

where

$$\hat{\det}L_{\alpha\beta}=\prod_{A=l+2}^{n}\lambda_{(A)}\ ,$$

where $\lambda_{(A)}$ are the nonzero eigenvalues of $L_{\alpha\beta}$; here there are $l+1$ zero eigenvalues, l occurring because we have assumed l conservation laws, and 1 occurring because we have assumed that there is one, and only one, Jacobi field with vanishing boundary conditions. The term $I(\nu,c)$ in I is

$$I(\nu,c)=\int_{\mathbb{R}}du\,\exp\left[i\left[cu-\frac{\nu}{3}u^3\right]\right]\ ,$$

where

$$c=-\frac{1}{\hbar}(p_f^{\Delta}-p_f)^{\alpha}\psi_{(1)\alpha}(\infty)\ , \tag{4.17}$$

and

$$\nu=-\frac{1}{2\hbar}\mathscr{V}_{111}=-\tfrac{1}{2}\int_{-\infty}^{+\infty}V_{,\alpha\beta\gamma}(q(t))\psi^{\alpha}_{(1)}(t)\psi^{\beta}_{(1)}(t)\psi^{\gamma}_{(1)}(t)dt\ . \tag{4.18}$$

The computation of ν is similar to the one performed in Sec. III C for the three other cases. Here the one-parameter family $\{q(\alpha)\}$ of classical paths is such that

$$\begin{aligned}
&q(\alpha_0)\text{ is the path defined by }(p_i,-\infty)(p_f,\infty)\ ,\\
&\partial q(\alpha)/\partial\alpha\,|_{\alpha_0}=\psi_{(1)}\text{ is the Jacobi field such that }\dot\psi_{(1)}(-\infty)=\dot\psi_{(1)}(\infty)=0\ ,\\
&\dot q(-\infty,\alpha)=p_i\text{ for all }\alpha\text{ and }q(-\infty,\alpha)=\alpha\partial q(-\infty,\alpha_0)/\partial\alpha_0,\text{ i.e. },\\
&\partial^2 q(-\infty,\alpha)/\partial\alpha^2=0\text{ and }\partial^2\dot q(-\infty,\alpha)/\partial\alpha^2=0\ .
\end{aligned} \tag{4.19}$$

$\partial^2 q(t,\alpha)/\partial\alpha^2$ satisfies the small disturbances of the small disturbance equation and can be solved with the Green's function of the Jacobi operator having the same boundary conditions:

$$\frac{\partial^2 q^{\mu}(t,\alpha)}{\partial\alpha^2}=-\frac{1}{m}\int_{-\infty}^{t}J^{\mu\sigma}(t,s)\nabla_\sigma\nabla_\mu\nabla_\rho V(q(s,\alpha))\psi^{\mu}_{(1)}(s)\psi^{\rho}_{(1)}(s)ds\ .$$

Taking the time derivative of both sides and setting $t=+\infty$, one obtains

$$\frac{\partial^2 \dot q^{\mu}(+\infty,\alpha)}{\partial\alpha^2}=-\frac{1}{m}\int_{-\infty}^{+\infty}\tilde K^{\mu\sigma}(\infty,s)V_{,\sigma\mu\rho}\psi^{\mu}_{(1)}(s)\psi^{\rho}_{(1)}(s)ds\ .$$

Taking the scalar product of both sides with $\psi^{\mu}_{(1)}(\infty)$ and using

$$\tilde K^{\mu\sigma}(\infty,s)\psi^{\mu}_{(1)}(\infty)=K^{\sigma\mu}(s,\infty)\psi^{\mu}_{(1)}(\infty)=\psi^{\sigma}_{(1)}(s)=\partial q^{\sigma}(s,\alpha_0)/\partial\alpha_0\ ,$$

one obtains

$$\nu=-\frac{1}{2\hbar}\left[\frac{\partial q}{\partial\alpha_0}(\infty,\alpha_0)\,\Bigg|\,\frac{\partial^2\dot q(\infty,\alpha_0)}{\partial{\alpha_0}^2}\right]\ . \tag{4.20}$$

In conclusion, the amplitudes for all four types of transitions in the Airy regime are

$$\mathscr{K}(\beta^{\Delta},t_b;\alpha,t_a)=\mathscr{C}\mathscr{D}^{-1/2}\exp\left[\frac{i}{\hbar}\varphi\right]I(\nu,c)\ , \tag{4.21}$$

where $\mathscr{C}$, $\mathscr{D}$, φ, and I are given in Table I. These quantities are obtained from one-parameter families of classical paths $\{q(\alpha)\}$ such that

$q(\alpha_0)$ is the classical path defined by $(\beta,t_b)(\alpha,t_a)$,

$\partial q(\alpha)/\partial\alpha\,|_{\alpha=\alpha_0}$ is the Jacobi field h with vanishing boundary values, hence the eigenvector $\psi_{(1)}$of the Jacobi operator with zero eigenvalue ,

$\partial^2 q(t_a,\alpha)/\partial\alpha^2=0$ and $\partial^2\dot q(t_a,\alpha)/\partial\alpha^2=0$.

In the case of momentum-to-momentum transitions,

TABLE I. The transition amplitudes in the Airy regime are [Eq. (4.21)] $\mathscr{K}(\beta^{\Delta},t_b;\alpha,t_a)=\mathscr{C}\mathscr{D}^{-1/2}\exp[(i/\hbar)\varphi]I(\nu,c)$. The values of $\mathscr{C}$, $\mathscr{D}$, φ, ν, and c for the four different amplitudes computed in this paper are listed in the table.

	Position to position	Momentum to position	Position to momentum	Momentum to momentum with l conservation laws
	$\mathscr{K}(b^{\Delta},t_b;a,t_a)$	$\mathscr{K}(b^{\Delta},t_b;p_i,-\infty)$	$\mathscr{K}(p_f^{\Delta},\infty;a,t_a)$	$\hat{\mathscr{K}}(p_f^{\Delta},\infty;p_i,-\infty)$
Boundary values of $h=\partial q/\partial\alpha_0$	$h(t_b)=h(t_a)=0$	$\dot{h}(-\infty)=h(t_b)=0$	$h(t_a)=\dot{h}(\infty)=0$	$\dot{h}(-\infty)=\dot{h}(\infty)=0$
The path q^{Δ} is defined by	$q^{\Delta}(t)=q(t)+(b^{\Delta}-b)\dfrac{t-t_a}{t_b-t_a}$	$q^{\Delta}(t)=q(t)+b^{\Delta}-b$	$q^{\Delta}(t)=q(t)+[(p_f^{\Delta}-p_f)/m](t-t_a)$	$q^{\Delta}(t)=q(t)+[(p_f^{\Delta}-p_f)/m]t$
φ where S is the action functional	$S(q^{\Delta},t_b,t_a)$	$S(q^{\Delta},t_b,-\infty)+\langle p_i,q^{\Delta}(-\infty)\rangle + \dfrac{1}{2m}\|p_i\|^2\int_{-\infty}^{t_b}dt$	$S(q^{\Delta},\infty,t_a)-\langle p_f^{\Delta},q^{\Delta}(\infty)\rangle + \dfrac{1}{2m}\|p_i\|^2\int_{t_a}^{\infty}dt$	$S(q^{\Delta},\infty,-\infty)+\langle p_i,q^{\Delta}(-\infty)\rangle - \langle p_f^{\Delta},q^{\Delta}(+\infty)\rangle+\int_{-\infty}^{\infty}E\,dt$
$\mathscr{D}$ in a system of coordinates where the 1 axis is perpendicular to the caustic	$\dfrac{\widehat{\det}_{\alpha\beta} J^{\alpha\beta}(t_b,t_a)}{\dot{h}^1(t_a)\dot{h}_1(t_b)}$ J given by (3.1), see also (A5) $\widehat{\det}$ defined by (3.15)	$\dfrac{\widehat{\det}_{\alpha\beta} K^{\alpha\beta}(t_b,-\infty)}{\dot{h}^1(-\infty)h_1(t_b)}$ K given by (3.2), see also (A6) $\widehat{\det}$ defined by (3.22)	$\dfrac{\widehat{\det}_{\alpha\beta} \tilde{K}^{\alpha\beta}(\infty,t_a)}{\dot{h}^1(t_a)h_1(t_b)}$ $\tilde{K}$ given by (3.3), see also (A11) $\widehat{\det}$ defined by (3.28)	$\dfrac{\widehat{\widehat{\det}}_{\alpha\beta} L_{\alpha\beta}(\infty,-\infty)}{h^1(-\infty)h_1(\infty)}$ L given by (3.4), see also (A12) $\widehat{\det}$ defined by (3.33) $\widehat{\widehat{\det}}$ defined by (4.16)
ν	$-\dfrac{1}{2\hbar}\left[\dfrac{\partial\dot{q}}{\partial\alpha_0}(t_b,\alpha_0)\middle\|\dfrac{\partial^2 q}{\partial\alpha_0{}^2}(t_b,\alpha_0)\right]$	$-\dfrac{1}{2\hbar}\left[\dfrac{\partial\dot{q}}{\partial\alpha_0}(t_b,\alpha_0)\middle\|\dfrac{\partial^2 q}{\partial\alpha_0{}^2}(t_b,\alpha_0)\right]$	$-\dfrac{1}{2\hbar}\left[\dfrac{\partial q}{\partial\alpha_0}(\infty,\alpha_0)\middle\|\dfrac{\partial^2 \dot{q}}{\partial\alpha_0{}^2}(\infty,\alpha_0)\right]$	$-\dfrac{1}{2\hbar}\left[\dfrac{\partial q}{\partial\alpha_0}(\infty,\alpha_0)\middle\|\dfrac{\partial^2 \dot{q}}{\partial\alpha_0}(\infty,\alpha_0)\right]$
c	$\hbar^{-1}\langle(b^{\Delta}-b)\mid\dot{h}(t_b)\rangle$	$\hbar^{-1}\langle(b^{\Delta}-b)\mid\dot{h}(t_b)\rangle$	$m^{-1}h^{-1}\langle p_f^{\Delta}-p_f\mid h(\infty)\rangle$	$m^{-1}h^{-1}\langle p_f^{\Delta}-p_f\mid h(\infty)\rangle$
$\mathscr{C}$	$-i(2\pi i\hbar)^{-(n+1)/2}$	$-i(2\pi i\hbar)^{-1/2}$	$-i(2\pi i\hbar)^{-1/2}$	$-i(2\pi i\hbar)^{(n-l-1)/2}$

$$\mathscr{K}(p_f^{\Delta},\infty;p_i,-\infty)=(2\pi\hbar)^l\delta(c_1)\cdots(c_l)\hat{\mathscr{K}}(p_f^{\Delta},\infty;p_i,-\infty)\ ,$$

it is obviously $\hat{\mathscr{K}}$ and not $\mathscr{K}$ which is of the form (4.21). The determinants $\mathscr{D}$ are all finite. In the first three cases they are finite because of the properties of the Jacobi operators having zero eigenvalues [Sec. III B Eqs. (3.14), (3.22), and (3.28)].

In the fourth case, it is finite because of two entirely different reasons:

(a) one similar to the previous case (3.33),

(b) one analyzed in the first paper of this series,[2]

In case (a), we had to deal with an isolated degenerate critical point of the *action functional* defined on the space of paths. In case (b), we had to deal with a submanifold of degenerate critical points of the sum of the *action functions* defined on the configuration space. In case (a), the critical point is degenerate because a projection of the phase-space flow of classical paths is caustic forming. In case (b), the critical points are degenerate because the action functional is invariant under a continuous group of transformations.

D. Comparison with the Schrödinger formalism

(i) We shall compare the WKB approximations of $\mathscr{K}(p_f,\infty;p_i,-\infty)$ and of the S-matrix element $\langle p_f \mid S \mid p_i \rangle$, obtained in the Schrödinger formalism, using the results of Landau and Lifshitz,[25] Mott and Massey,[26] Newton,[27] and Schiff.[28] It can be shown[28] that

$$\langle p_f \mid S \mid p_i \rangle = \mid p_i \mid^{-2}\delta(\mid p_f\mid - \mid p_i \mid)\left[\frac{1}{\sin\theta_i}\delta(\theta_f-\theta_i)\delta(\phi_f-\phi_i)+\frac{i}{2\pi}\mid p_i\mid f(p_f,p_i)\right]$$

$$=\frac{1}{2\pi}\exp(i\pi/2)\mid p_i\mid^{-1}f(p_f,p_i)\delta(\mid p_f\mid-\mid p_i\mid)\ \text{for}\ \theta_f\neq\theta_i\ \text{and}\ \phi_f\neq\phi_i\ , \tag{4.22}$$

where the polar coordinates of p are $\{\mid p\mid,\theta,\phi\}$ and where $f(p_f,p_i)$ is the usual scattering amplitude. If the potential V is spherically symmetric, the scattering amplitude $f(\theta)$ is given in terms of the phase shifts by the Raleigh-Faxen-Holtsmark formula

$$f(\theta)=\frac{1}{2k}\exp(-i\pi/2)\times\sum_{l=0}^{\infty}(2l+1)[\exp(2i\delta_l)-1]P_l(\cos\theta)\ , \tag{4.23}$$

where

$$\hbar^2k^2=\mid p_i\mid^2=\mid p_f\mid^2=2mE\ ,$$

$P_l(\cos\theta)$ are the Legendre polynomials, and the phase shifts δ_l are defined by the asymptotic form of the wave function

$$\psi\approx\sum_l A_lP_l(\cos\theta)(kr)^{-1}\sin(kr-l\pi/2+\delta_l)\ . \tag{4.24}$$

The formula (4.22) is obtained by subtracting the contribution of the initial wave function from the asymptotic value of the solution of the Schrödinger equation equal to a plane wave of momentum p_i as $t\to-\infty$. But, in fact, one subtracts it only partially because one argues that (4.23) can be replaced by

$$f(\theta)=\frac{1}{2k}\exp(-i\pi/2)\sum_{l=0}^{\infty}(2l+1)\exp(2i\delta_l)P_l(\cos\theta) \tag{4.25}$$

on the grounds that it invalidates the result only for $\cos\theta=1$. The terms in (4.23) missing in (4.25) can be traced back to the initial wave function, hence the initial wave function is only partially subtracted.

The WKB approximation of $f(\theta)$ is obtained by computing the asymptotic value of (4.23) for large l. Thus one uses

$$\delta_l\approx\int_{r_0}^{\infty}(F^{1/2}-k)dr-kr_0+\pi/4-l\pi/2\ , \tag{4.26}$$

where r_0 is the radial distance to the point of closest approach, and

$$F=k^2-2m\hbar^{-2}V(r)-(l+\tfrac{1}{2})^2r^{-2} \tag{4.27}$$

For large l the eigenvalues $\hbar[l(l+1)]^{1/2}\equiv M$ of the angular momentum operator are approximated[29] by

$$M\approx\hbar l\ \text{or}\ M\approx\hbar(l+\tfrac{1}{2})\ . \tag{4.28}$$

The asymptotic values of $P_l(\cos\theta)$ for large l is

$$P_l(\cos\theta)\approx-(2\pi l\sin\theta)^{-1/2}\exp(i\pi/2)\{\exp[i(l+\tfrac{1}{2})\theta+i\pi/4]-\exp[-i(l+1/2)\theta-i\pi/4]\}\ . \tag{4.29}$$

Finally, one replaces $f(\theta)$ by its stationary-phase approximation. The critical value l_0 of l for the first term satisfies the equation

$$2\,\partial\delta_l/\partial l\mid_{l=l_0}+\theta=0 \tag{4.30}$$

and the critical value l_0 of l for the second terms satisfies

$$2\,\partial\delta_l/\partial l\mid_{l=l_0}-\theta=0\ . \tag{4.31}$$

Using for δ_l its asymptotic value (4.26), Eqs. (4.30) and (4.31) are satisfied if

$$-2\int_{r_0}^{\infty}dr\,Mr^{-2}\{2m[E-V(r)]-M^2r^{-2}\}^{-1/2}-\pi\pm\theta=0\ . \tag{4.32}$$

This equation is identical with the equation of classical mechanics which gives the classical scattering angle θ as a function of the classical angular momentum. It can be solved for M with the positive sign if the potential is attractive and with the negative sign if the potential is repulsive. We shall assume the potential to be repulsive, hence (4.30) has no solution and the first term does not contribute[30] to $f_{\rm WKB}(\theta)$. If we identify the eigenvalue of the angular momentum operator with its classical value, then $\hbar l_0$ is the classical angular momentum M corresponding to the classical scattering angle θ, and we can write

$$f_{\rm WKB}(\theta)=|f_{\rm WKB}(\theta)|\exp(2i\beta_{\rm WKB}) \tag{4.33}$$

with

$$\begin{aligned}|f_{\rm WKB}(\theta)| &\approx \frac{2M+1}{2k}(2\pi M\sin\theta)^{-1/2}\\ &\quad\times(2\pi)^{1/2}(\partial\theta/\partial M)^{-1/2}\\ &\approx (M/2mE)^{1/2}(\sin\theta\,\partial\theta/\partial M)^{-1/2}\end{aligned} \tag{4.34}$$

and

$$2\beta_{\rm WKB}=2\delta_M-2(M+\tfrac{1}{2})\partial\delta_M/\partial M-\tfrac{1}{2}\pi\ . \tag{4.35}$$

Inserting (4.26) into (4.35), one obtains

$$\begin{aligned}2\beta_{\rm WKB} &= -2kr_0+2\hbar^{-2}\int_{r_0}^{\infty}2m(E-V)F^{-1/2}dr\\ &\quad -2k\,|_{r_0}^{\infty}\\ &=\lim_{R\to\infty}2\hbar^{-1}\int_{r_0}^{R}2m(E-V)F^{-1/2}dr-2kR\\ &=\lim_{R\to\infty}2\hbar^{-1}\left[\int_{t_0}^{t_R}2(E-V)dt-(2mE)^{1/2}R\right]\\ &=\lim_{R\to\infty}2\hbar^{-1}\left[\int_{t_0}^{t_R}L\,dt+E(t_R-t_0)\right.\\ &\qquad\left.-(2mE)^{1/2}R\right]\\ &=\lim_{t_a\to-\infty,t_b\to\infty}\left[S(p_f,t_b;p_i,t_a)\right.\\ &\qquad\left.+\int_{t_a}^{t_b}E\,dt\right]\ .\end{aligned} \tag{4.36}$$

We have already shown [(4.10) and (4.12)] that this limit is finite for potentials $V(r)$ decreasing faster than r^{-1} at infinity.

In conclusion, according to (4.34) and (4.36) on the one hand, and Eq. (44), paper I and (4.9) on the other hand,

$$\mathscr{K}_{\rm WKB}(p_f,+\infty,p_i,-\infty)=\langle p_f\,|\,S\,|\,p_i\rangle_{\rm WKB}\ . \tag{4.37}$$

Remark. There are two sources of confusion which sometimes lead to erroneous statements concerning the WKB approximation of the S matrix.

(i) $\delta_{\rm WKB}$ is sometime confused with $\beta_{\rm WKB}$. (ii) For momentum-to-momentum transitions, the action function (i.e., the generator of canonical transformations) is not equal to the action functional (i.e., the integral of the Lagrangian along the classical path defined by the momenta), but to the action functional *plus* appropriate end-point contributions (Ref. 2, Appendix).

(ii) We shall compare the Airy regime of $\mathscr{K}(p_f,\infty;p_i,-\infty)$ with the results derived by Ford and Wheeler for spherically symmetric potentials.[31] They examine the cases where $\partial\theta/\partial M=2\,\partial^2\delta_M/\partial M^2=0$ (rainbow), $\sin\theta(M)=0$ (glory), $\theta(M)$ is singular (orbiting), and $\theta(M)$ is multivalued (interferences). In the first three cases, they expand $\theta(M)$ around the appropriate value of M, integrate the equation $2\,\partial\delta_M/\partial M=\theta(M)$, and analyze the corresponding scattering amplitudes.

We shall compute the Airy function $I(\nu,c)$ of $\mathscr{K}(p_f,\infty;p_i,-\infty)$ explicitly when V is a spherically symmetric potential. According to the method outlined in subsection C, we construct a one-parameter family of classical paths $\{q(\alpha){:}\alpha=\beta\}$ parametrized by the impact parameter B which satisfies the conditions (4.19) [we use $q(B)(t)=q(t,B)$]:

$q(B_0)$ is the path defined by

$$(p_i,-\infty)(p_f,\infty)\ ,$$

$\partial q(B)/\partial B\big|_{B=B_0}=\psi$ is the Jacobi field such that $\dot\psi(-\infty)=\dot\psi(\infty)=0$,

$\dot q(-\infty,B)=p_i$ for all B and

$$q(-\infty,B)=\lim_{t_a\to-\infty}q(t_a,B)\ ,$$

where $q(t_a,B)$ is given in cylindrical coordinates by (z_a,B,ϕ) .

It follows that $\partial q(t_a,B)/\partial B=(0,1,0)$ and $\partial^2q(t_a,B)/\partial B^2=(0,0,0)$. By virtue of (4.20), the scaling factor ν of the Airy function is

$$\nu=-\frac{1}{2\hbar}\lim_{t_b\to\infty}\psi_\mu(t_b)\partial^2q^\mu(t_b,B)/\partial B^2\ . \tag{4.38}$$

Let θ_0 be the caustic angle, i.e., the classical scattering angle corresponding to the impact parameter B_0 such that

$$\partial\theta/\partial B\big|_{B=B_0}=0\ .$$

A nearby scattering angle θ can be written

$$\theta=\theta_0+\tfrac{1}{2}(B-B_0)^2\partial^2\theta/\partial B^2+\cdots\ . \tag{4.39}$$

For large values of t_b we choose the following axes: the z axis makes an angle θ_0 with the direction of the initial momentum p_i, the x axis is perpendicular to the z axis in the plane of motion, the y axis completes the coordinate system to make an orthonormal frame. Then

$$\begin{aligned}m\dot q^{(z)}(\infty,B)&=|p_f|\cos(\theta-\theta_0)=|p_f|\{1-\tfrac{1}{2}[\tfrac{1}{2}(B-B_0)^2\partial^2\theta/\partial B^2]^2+\cdots\}\ ,\\ m\dot q^{(x)}(\infty,B)&=|p_f|\sin(\theta-\theta_0)=|p_f|[\tfrac{1}{2}(B-B_0)^2\partial^2\theta/\partial B_0{}^2+\cdots]\ ,\\ \dot q^{(y)}(\infty,B)&=0\ .\end{aligned} \tag{4.40}$$

Hence

$$\partial^2 \dot{q}^{(z)}(\infty, B)/\partial B^2 \Big|_{B=B_0} = 0$$

$$m\, \partial^2 \dot{q}^{(x)}(\infty, B)/\partial B^2 \Big|_{B=B_0} = |p_f|\, \partial^2\theta/\partial B^2 \Big|_{B=B_0} . \tag{4.41}$$

Moreover, $\psi^{(x)}(\infty) = \partial q^{(x)}(\infty, B)/\partial B = 1$; thus

$$\nu = -\frac{1}{2\hbar m} |p_f|\, \partial^2\theta/\partial B^2 \Big|_{B=B_0} . \tag{4.42}$$

Thus, if

$$\partial\theta/\partial B \Big|_{B=B_0} = 0 ,$$

i.e., if $\partial^2 \delta_M/\partial M^2 = 0$, the transition amplitude $\mathscr{K}(p_f^{\Delta}, \infty; p_i, -\infty)$ is proportional to an Airy function $I(\nu, c)$ with

$$\left.\begin{aligned} c &= \frac{1}{\hbar m}(p_f^{\Delta} - p_f)^{(x)} \\ \nu &= \frac{1}{2\hbar m} |p_f|\, \partial^2\theta/\partial B^2 \,|_{B=B_0} \end{aligned}\right\} \text{for the x axis perpendicular to the z axis asymptotic to the rainbow path .}$$

This is the result obtained by Ford and Wheeler for rainbow scattering by spherically symmetric potentials. In addition, (4.41) gives an explicit value for $\partial^2\theta/\partial B^2$.

E. Comparisons with other path-integral results

Because it bypasses the circuitous route "partial-wave decomposition followed by stationary phase approximation for the summation over l", the path-integral formalism is a natural vehicle for the computation of semiclassical expansions of scattering amplitude.[32] Previous path-integral calculations have been hampered by one or the other of the following issues which have since been resolved.

(1) The role of classical conservation laws in semiclassical approximations of path integrals.

(2) The caustic problem for scattering theory using momentum-to-momentum amplitudes. Without a Feynman-Kac formula for such amplitudes, one had to approach the caustic problem in terms of position-to-position, or momentum-to-position amplitudes.

V. CONCLUSION

The intuitive character of the path-integration formalism has been widely exploited for the analysis of WKB approximations. If the path integrals are expressed in terms of Gaussian integrators whose covariance is the appropriate Green's function of the Jacobi operator of the system, the path-integral formalism has the same intuitive character for the analysis of the Airy regime. We can now relate the successive terms in a power expansion in $\hbar_{1/2}$ to a more and more refined analysis of the classical flow corresponding to the initial wave function:

Terms of order $\hbar^{-1}$ are obtained from a classical path q.

Terms of order $\hbar^{-1/2}$ give no contribution by virtue of the Euler-Lagrange equation.

Terms of order $\hbar^0$ are obtained from a Jacobi field h along q.

Terms of order $\hbar^{1/2}$ are obtained from the solutions of the small disturbances of the Jacobi operator.

These latter terms occur in different contexts:

Momentum-to-position transitions expressed in terms of the $\widetilde{K}$ matrix, momentum-to-momentum transitions expressed in terms of the L-matrix, and Airy regime of all types of transitions.

Since a caustic is signaled by the existence of a nonzero Jacobi field with vanishing boundary conditions, the explicit appearance of the Jacobi fields in the covariance of the integrator makes the calculation of caustics intuitively clear.

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This investigation began as a first step in the analysis of numerical results obtained by R. Matzner for the scattering of gravitational waves by black holes. J. A. Wheeler noticed that the cross sections exhibit some features of glory scattering. This remark raised new issues in the theory of gravitational-wave scattering which might be answered by path-integration techniques. Hence the present paper. Why the study of caustics in quantum mechanics will shed light on the study of glories in classical wave scattering may be intuitively familiar, but a careful justification requires another paper which will be published in due time. At this point we want only to thank Richard Matzner and John Wheeler for stimulating discussions, and John Futterman for clarifications of the gravitational wave-scattering problem. We thank Alice Young for her drawing of the Jacobi fields along Coulomb paths and her critical study of several phase shift calculations. This work was begun at the Institute for Theoretical Physics (Santa Barbara), continued during a second visit at the ITP, and mostly completed at the Institut des Hautes Etudes Scientifiques (Bures-sur-Yvette). We thank these institutes as well as our home institutions for having provided excellent working conditions. We thank the Institute of Theoretical Physics, Academia Sinica, for having made it possible for one of us (Z.T.-R.) to come to the University of Texas at Austin. This work was supported in part by NSF Grants Nos. PHY81-07381, PHY81-06909, and PHY78-26592.

*Now at Bell Laboratories, WB 1A-216, Holmdel, New Jersey 07733.

[1]C. DeWitt-Morette, A. Maheshwari, and B. Nelson, Phys. Rep. 50, 255 (1979).

[2]See the Appendix in C. DeWitt-Morette and T.-R. Zhang, second preceding paper, Phys. Rev. D 28, 2503 (1983).

[3]We use the word "integrator" generically for a measure, a promeasure, a prodistribution, etc., γ which, together with an integrand f, defines an integral $I=\int f(x)d\gamma(x)$.

[4]K. W. Ford and J. A. Wheeler, Ann. Phys. (N.Y.) 7, 259 (1959).

[5]N. F. Mott and H. S. W. Massey, *The Theory of Atomic Collisions,* 3rd ed. (Oxford University Press, London, 1965).

[6]L. S. Schulman, in *Functional Integration and its Applications,* edited by A. M. Arthur (Clarendon, Oxford, 1975); see also Ref. 32.

[7]J. H. Van Vleck, Proc. Nat. Acad. Sci. U.S.A. 14, 178 (1928). In non-Cartesian coordinates, it has been shown in Ref. 1, p. 299 that the right-hand side of (2.6) is multiplied by $|\det_{\alpha\beta}g_{\alpha\beta}(\bar{q}(t_a))|^{1/4}|\det_{\alpha\beta}g_{\alpha\beta}(\bar{q}(t))|^{-1/4}$.

[8]W. Gordon, Z. Phys. 48, 180 (1928). Translation and illustrations by A. Young, Center for Relativity, University of Texas at Austin, 1982.

[9]See, for instance, in Ref. 11, p. 353, three equivalent definitions of caustics, (1) as an envelope of a family of classical paths; (2) as a set of conjugate points along a classical path characterized by nonzero Jacobi fields with vanishing boundary conditions; or (3) characterized by $2n$ Jacobi fields which are not linearly independent.

[10]See Ref. 2, Appendix. See also K. D. Elworthy and A. Truman, J. Math. Phys. 22, 2144 (1981).

[11]See, in Ref. 1, detailed calculations of (A45) and (A46) for the two types of initial wave functions considered here.

[12]C. DeWitt-Morette and T.-R. Zhang, preceding paper, Phys. Rev. D 28, 2517 (1983).

[13]B. Nelson, Phys. Rev. D 27, 841 (1983).

[14]See Ref. 2, Appendix. Their definitions and properties. See also (2.3).

[15]C. DeWitt-Morette, Ann. Phys. (N.Y.) 97, 367 (1976). See also Ref. 2, Appendix.

[16]See Ref. 1, p. 358.

[17]A summary of the properties of the Airy function can be found in Appendix B of L. D. Landau and E. M. Lifshitz, *Quantum Mechanics,* 3rd ed. (Pergamon, Oxford, 1977).

[18]The Airy regime for position-to-position transitions has partially been done in Ref. 1. See Ref. 1 for the details of the calculation, in particular, see pp. 282, 283, 310, 311, and 316 for how the integrators $w_\pm$ induce an integrator w on the space of paths with both ends fixed.

[19]Since we have assumed that the Jacobi operator has only one zero eigenvalue, there are at most two classical paths defined by the given boundary conditions.

[20]The quantity called Δ in Ref. 1 is equal to Δ/μ in this paper. The new change of variable (3.35) keeps a clearer distinction between the two independent limits $\hbar$ tending to zero and b^Δ tending to b.

[21]The same calculation can be done for arbitrary Lagrangians defined on Riemannian manifolds. See Ref. 1 for Riemannian configuration spaces; for velocity-dependent potentials and for time-dependent metrics, see B. Nelson and B. Sheeks, J. Math. Phys. 22, 1944 (1981); Commun. Math. Phys. 84, 515 (1982).

[22]"Limit $\hbar\to 0$" is to be understood as "the dominating term when $\hbar$ tends to zero." The dominating term is always proportional to some positive power of $\hbar$, so that strictly speaking, the right-hand side of (4.1) vanishes for $\hbar\to 0$.

[23]See Ref. 2, Appendix for the expression of the action function when the path is characterized by initial and final momenta.

[24]For a discussion of systems which approach integrable systems asymptotically, see W. Thirring, *Classical Dynamical Systems* (Springer, New York, 1978).

[25]See Landau and Lifshitz, *Quantum Mechanics,* Ref. 17, pp. 503—520.

[26]See Mott and Massey, *The Theory of Atomic Collisions,* Ref. 5, pp. 369—380.

[27]R. G. Newton, *Scattering Theory of Waves and Particles* (McGraw-Hill, New York, 1966), pp. 298—302, 572.

[28]L. I. Schiff, in *Quantum Mechanics,* Ref. 17, pp. 322 (37.31).

[29]These approximations are obviously valid for large l, but they are also made for not so large l. For a careful analysis of this procedure, see R. E. Langer, Phys. Rev. 51, 669 (1937).

[30]See, for instance, Ref. 2, Eq. (24).

[31]For a summary, see Mott and Massey, Ref. 5 pp. 102—110, and Landau and Lifshitz, Ref. 17, pp. 518—523.

[32]P. Pechukas, Phys. Rev. 181, 166 (1969). W. V. Berry and K. E. Mount, Rep. Prog. Phys. 35, 315 (1972); see also M. Berry, in *Physique des Défauts,* edited by R. Balian, M. Kleman, and J. P. Poirier (North-Holland, Amsterdam, 1981). L. S. Schulman, *Techniques and Applications of Path Integration* (Wiley-Interscience, New York, 1980). See also S. Levit and U. Smilansky, Ann. Phys. (N.Y.) 108, 165 (1977); S. Levit, in *Path Integrals and Their Applications,* edited by G. J. Papadopoulos and J. T. Devreese (Plenum, New York, 1978). K. Yajima, Commun. Math. Phys. 69, 101 (1979). Our own interest and approach has its origin in Schulman's work.