Path integrals and conservation laws

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If the initial and the final states of a system have classical limits, and if the classical limits cannot be chosen independently from each other without violating classical conservations laws, the JWKB approximation of the probability amplitude for the transition between such initial and final states requires special care. We compute it explicitly for momentum to momentum transitions and for angular momentum to angular momentum transitions. It is shown how the classical conservation laws make their appearance in the limit $\hbar=0$. The statements are illustrated by applications to potential scattering theory.

I. INTRODUCTION

In the operator formalism of quantum physics, a dynamical variable is a constant of the motion if it does not depend explicitly on time and if it commutes with the Hamiltonian of the system. The quantum concept of constant of the motion corresponds to the classical concept by the "commutator-Poisson bracket" correspondence. How are these basic ideas translated in the path-integral formalism of quantum physics? Somehow the WKB calculations must give vanishingly small values to probabilities for transitions between states whose classical limits are incompatible because they violate the constraints imposed on them by the classical conservation laws. For example, let $\mathscr{K}(p_b,t_b;x,t)$ be the probability amplitude that a particle being at $x\in M$ at time $t\in T=[t_a,t_b]$ be found with the momentum p_b at time t_b, and let $\mathscr{K}(x,t;p_a,t_a)$ be defined similarly. What is the quantity

$$\mathscr{K}(p_b,t_b;p_a,t_a)\equiv\int_M dx\,\mathscr{K}(p_b,t_b;x,t)\mathscr{K}(x,t;p_a,t_a)\ ? \tag{1}$$

It often happens that p_a and p_b can be treated as independent variables on the right-hand side of (1), but that they have to be treated as constrained variables on the left-hand side because of conservation laws. We shall show that in the limit $\hbar=0$, the integrations in (1) bring out the conservation laws. Mathematically, the problem is the calculation of an integral by the stationary-phase approximation when the set of critical points, all of which are degenerate, form a submanifold of M.

Indeed the critical points of the action functional $\underline{S}$ defined on the space X of paths $f:T\to M$ are the solutions of the Euler-Lagrange equation. Let $q(p_a,p_b)$ be a solution of the Euler-Lagrange equation characterized by its initial and final momenta. If $\underline{S}$ is invariant under a continuous group G of transformations $\mathscr{F}$, then the critical values of $\underline{S}$ are constant on the submanifold $Y\subset X$ consisting of the paths $q(\mathscr{F}p_a,\mathscr{F}p_b)$ for any $\mathscr{F}\in G$.

II. WKB AMPLITUDES SUBJECT TO CONSERVATION LAWS (REF. 1)

We shall compute the WKB approximation of $\mathscr{K}(p_b,t_b;p_a,t_a)$ defined by (1) for the system

$$L(q,\dot q)=\tfrac{1}{2}m\,|\,\dot q\,|^2-V(q) \tag{2}$$

defined[2] on $M=R^n$. That is, we shall compute[3]

$$I\equiv\mathscr{K}_{\rm WKB}(p_b,t_b;p_a,t_a)\equiv\lim_{\hbar=0}\int_M dx\,\mathscr{K}_{\rm WKB}(p_b,t_b;x,t)\mathscr{K}_{\rm WKB}(x,t;p_a,t_a)\ , \tag{3}$$

where $\mathscr{K}_{\rm WKB}(x,t;p_a,t_a)$ is the WKB approximation of

$$\mathscr{K}(x,t;\phi_a,t_a)=\int_{Y_+}dw_+^W(y)\exp\left[-\frac{i}{\hbar}\int_{t_a}^{t}V(x+\mu y(s))ds\right]\times\phi_a(x+\mu y(t_a)) \tag{4}$$

for ϕ_a a plane wave of momentum p_a, and $\mathscr{K}_{\rm WKB}(p_b,t_b;x,t)$ is the WKB approximation of

$$\mathscr{K}(\phi_b,t_b;x,t)=\int_{Y_-}dw_-^W(y)\exp\left[-\frac{i}{\hbar}\int_{t}^{t_b}V(x+\mu y(s))ds\right]\times\phi_b^*(x+\mu y(t_b)) \tag{5}$$

for ϕ_b a plane wave of momentum p_b, where $\mu=(\hbar/m)^{1/2}$, Y_-, and Y_+ are the spaces of continuous paths vanishing, respectively, at t_a and t_b, w_-^W, and w_+^W are the complex Wiener integrators defined by their Fourier transforms

$$(\mathscr{F}w_\mp^W)(\mu)=\exp\left[-\frac{i}{2}\int_T d\mu_\alpha(t)\int_T d\mu_\beta(s)G_\mp^{W\alpha\beta}(t,s)\right]\ , \tag{6}$$

$$G_-^W(t,s) = \inf(t-t_a, s-t_a)\mathbb{1},$$
$$G_+^W(t,s) = \inf(t_b-t, t_b-s)\mathbb{1}\ . \tag{7}$$

The initial and final wave functions are chosen[4] to be

$$\phi_a = \exp\left[\frac{i}{\hbar}S_a\right]T_a\ , \text{ and similarly for } \phi_b\ , \tag{8}$$

where S_a,S_b, T_a, and T_b are well-behaved functions on the configuration space. The support of T_a or T_b determines the localization of the system. The associated classical problem[4] to the quantum system (4) [(5)] is the flow of classical trajectories of (2) with boundary conditions at $t=t_a$ [at $t=t_b$],

$$p_a(x) = \nabla S_a(x)\ \ [p_b(x) = \nabla S_b(x)]\ . \tag{9}$$

If the classical flow is a one-one mapping[5] on the domain of the wave function, then[6]

$$\mathscr{K}_{\rm WKB}(x,t;\phi_a,t_a) = \exp\left[\frac{i}{\hbar}S(x,t;p_a,t_a)\right] \times |\det \partial^2 S(x,t;p_a,t_a)/\partial x^\beta \partial p_{a\alpha}|^{1/2} T_a(q_a(t_a))\ , \tag{10}$$

$$\mathscr{K}_{\rm WKB}(\phi_b,t_b;x,t) = \exp\left[\frac{i}{\hbar}S(p_b,t_b;x,t)\right] \times |\det \partial^2 S(p_b,t_b;x,t)/\partial p_{b\beta}\partial x^\alpha|^{1/2} T_b(q_b(t_b))\ , \tag{11}$$

where the action functions are defined by the action functional

$$\underline{S}(q) = \int_T L(q(t),\dot{q}(t))dt$$

and the endpoint contributions introduced by the initial or final wave function:

$$S(x,t;p_a,t_a) = \underline{S}(q_a) + S_a(q_a(t_a)) \text{ for } q_a \text{ the classical path defined by } (p_a,t_a)(x,t)\ , \tag{12}$$

$$S(p_b,t_b;x,t) = \underline{S}(q_b) - S_b(q_b(t_b)) \text{ for } q_b \text{ the classical path defined by } (x,t)(p_b,t_b)\ . \tag{13}$$

The expression "the classical path defined by $(p_a,t_a)(x,t)$" is to be understood as follows (see Fig. 1). Let $\Phi_s: M \to M$ be the classical flow defined by

$$\ddot{\Phi}_s(a) = -\nabla V(\Phi_s(a)) \text{ with } \ddot{\Phi}_s = d^2\Phi_s/ds^2\ ,$$
$$\Phi_0(a) = a,\quad \dot{\Phi}_0(a) = \nabla S_a(a)\ ; \tag{14}$$

then the classical path defined by $(p_a,t_a)(x,t)$ is

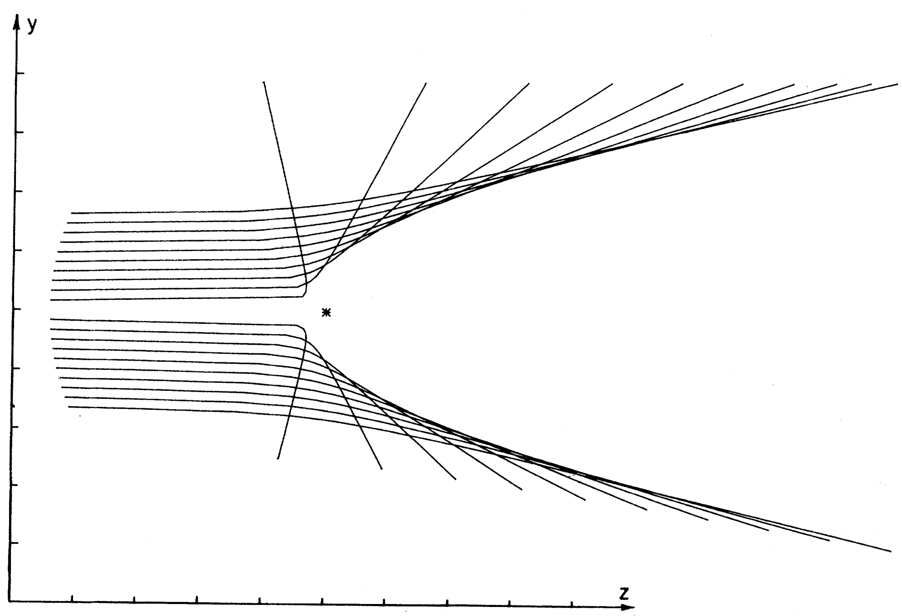

FIG. 1. Family of classical paths having the same initial momentum at $t_a = -\infty$ in a repulsive Coulomb potential. Let $A \equiv eE/mv_0^2$, $B \equiv$ impact parameter. For a given A, the B family of Coulomb paths satisfy $B(y-B) = A[z+(z^2+y^2)^{1/2}]$ in the $y-z$ plane with the potential at the origin of the coordinates. This flow is caustic forming in configuration space, but is not caustic forming in momentum space. For A negative (attractive potential), the flow is not caustic forming (Ref. 7).

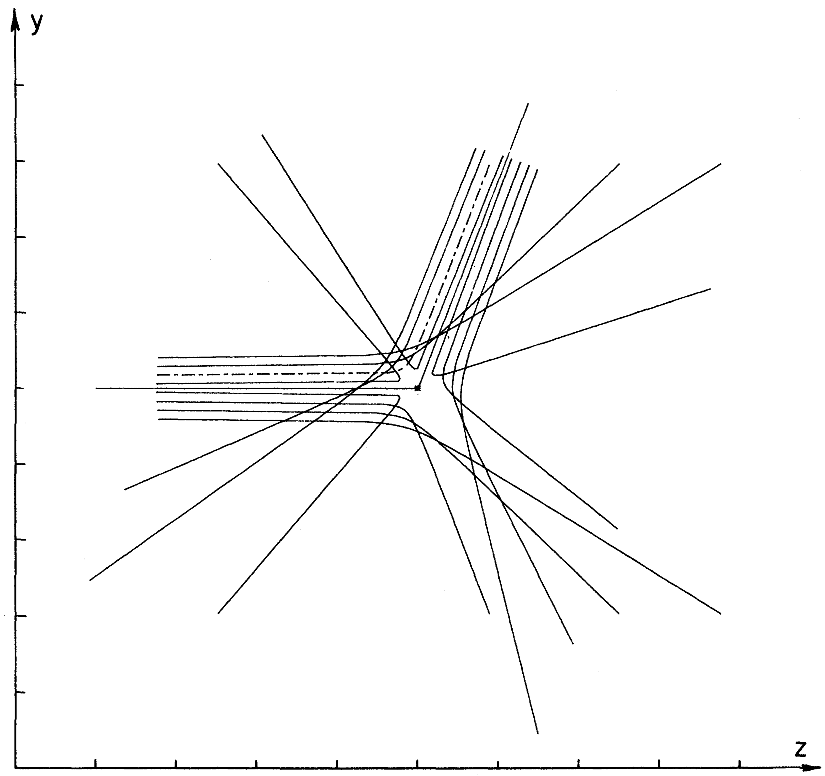

FIG. 2. Two classical flows of Coulomb paths: one having the same initial momentum p_a at $t_a=-\infty$ in the z direction, the other having the same final momentum p_b at $t_b=+\infty$ in a direction making an angle $\theta=70°$ with the z direction. The norms of p_a and p_b are equal, and there is one path (the dot-dash line) which belongs to both flows.

$$\Phi_{s-t_a}\circ\Phi^{-1}_{t-t_a}(x)\ . \tag{15}$$

The classical path defined by $(x,t)(p_b,t_b)$ is

$$\Psi_{s-t_b}\circ\Psi^{-1}_{t-t_b}(x)\ , \tag{16}$$

where Ψ_s is the classical flow defined by

$$\ddot{\Psi}_s(b)=-\nabla V(\Psi_s(b))\ ,\quad \Psi_0(b)=b,\ \ \dot{\Psi}_0(b)=\nabla S_b(b)\ . \tag{17}$$

A path can belong to both flows (see Fig. 2) if there is a point x_0 and a time t_0 such that

$$\Psi_{t-t_b}\circ\Psi^{-1}_{t_0-t_b}(x_0)=\Phi_{t-t_a}\circ\Phi^{-1}_{t_0-t_a}(x_0)\ . \tag{18}$$

With the WKB approximations being given by (10) and (11), Eq. (3) can be written

$$I\equiv\lim_{\hbar=0}\int_{R^n}dx\,\exp\left[\frac{i}{\hbar}F(x)\right]A(x) \tag{19}$$

with

$$F(x)\equiv S(p_b,t_b;x,t)+S(x,t;p_a,t_a)\ , \tag{20}$$

$$A(x)\equiv|\det_{\alpha\beta}\partial^2S(p_b,t_b;x,t)/\partial p_{b\beta}\partial x^{\alpha}|^{1/2}\,|\det_{\alpha\beta}\partial^2S(x,t;p_a,t_a)/\partial x^{\beta}\partial p_{a\alpha}|^{1/2}T_a(q_a(t_a))T_b(q_b(t_b))\ . \tag{21}$$

The critical points x_0 of F satisfy the equations

$$\partial F(x_0)/\partial x_0^{\alpha}\equiv F_{,\alpha}(x_0)=0,\quad \alpha=1,\dots,n\ . \tag{22}$$

The x^{α} derivative of the action function defined by (12) [by (13)] is[8] the momentum $p_{a\alpha}(t)$ along the classical q_a [minus the momentum $p_{b\alpha}(t)$ along the classical path q_b]. Equations (22) say that if x_0 is a critical point,

$$p_{a\alpha}(t)=p_{b\alpha}(t)\ . \tag{23}$$

Equations (23) are satisfied if and only if the homotopic product path[9] $q\equiv q_bq_a$ is a classical path, that is to say if q belongs both to the flow (15) and to the flow (16). We shall say in brief that q is defined by $(p_a,t_a)(p_b,t_b)$. We have two cases to consider according to whether or not $F_{,\alpha}(x_0)=0$ has a solution on the support of A.

(1) There is no classical path q belonging to both flows. Then, for T_a or T_b of compact support, I tends to zero faster than any power of $\hbar$

$$I=O(\hbar^n)\ \text{for } n \text{ an arbitrary integer}\ . \tag{24}$$

The essence of the proof of this well-known result can be stated for the one-dimensional integral

$$\int_R dx\, A(x)\exp\left[\frac{i}{\hbar}F(x)\right]=\int_R dx\, A(x)\left[\frac{i}{\hbar}\frac{\partial F}{\partial x}\right]^{-1}\frac{d}{dx}\left[\exp\left[\frac{i}{\hbar}F(x)\right]\right],\ \text{for } \partial F/\partial x\neq 0 \text{ on supp} A\ ,$$
$$=i\hbar\int_R dx\frac{d}{dx}\left[A(x)\left[\frac{\partial F}{\partial x}\right]^{-1}\right]\exp\left[\frac{i}{\hbar}F(x)\right], \tag{25}$$

since A is of compact support. By repeated usage of integration by parts one obtains (24). Q.E.D.

In the limit $\hbar=0$, the probability amplitude for finding in the state ϕ_b at t_b the system known to be in the state ϕ_a at t_a vanishes if there is no classical path belonging both to the classical flows defined by ϕ_a and ϕ_b.

(2) There is at least one classical path q belonging to both flows. If Eqs. (22) have a solution, they are likely to have an infinite number of solutions, namely any point x_0 on a path belonging to both flows. We shall assume that there is only one classical path belonging to both flows.[5]

If, for instance, $p_{a1}(t)$ and $p_{b1}(t)$ are constant and equal, respectively, to $p_{a1}(t_a)$ and $p_{b1}(t_b)$, then Eq. (23) says $p_{a1}(t_a)=p_{b1}(t_b)$. This equation does not impose a condition on x_0 but a constraint on the choice of initial and final states. We shall refer, in brief, to such an equation as a "conservation equation". In general, possibly after a change of coordinates, the equations $F_{,\alpha}(x_0)=0$ split into

l conservation equations , (26a)

$n-l$ equations which determine n components of x_0 . (26b)

We shall assume that (26b) has a unique solution[5] for $n-l$ components of x_0, i.e., (26b) defines a connected l-dimensional submanifold $N\subset M$. Let $\{x^\alpha\}\to\{\bar{x}^\alpha\}$ be the change of coordinates, if any, which splits the set $\{F_{,\alpha}(x_0)\}$ into (26a) and (26b). Let $\bar{p}=\partial\bar{L}/\partial\bar{q}$ be the corresponding generalized momenta. Set $\bar{F}(\bar{x})=F(x(\bar{x}))$ and order the coordinates so that

$\bar{F}_{,a}=0,\ a=1,\ldots,l$ are the conservation equations , (27a)

$\bar{F}_{,A}=0,\ A=l+1,\ldots,n$ are the remaining equations . (27b)

It is now necessary to generalize the lemma of Morse.[10] Set

$$y=\bar{x}-\bar{x}_0\ ,\qquad G(y)=\bar{F}(y+\bar{x}_0)-S(p_b,t_b;p_a,t_a) \tag{28}$$

with

$$S(p_b,t_b;p_a,t_a)=S(p_b,t_b;x_0,t_0)+S(x_0,t_0;p_a,t_a)\ . \tag{29}$$

Lemma. There is a local system of coordinates in a neighborhood of $\bar{x}_0$ such that

$$G(y)=\sum_{a=1}^{l}y^a g_a-\tfrac{1}{2}\sum_{A=l+1}^{p}(y^A)^2+\tfrac{1}{2}\sum_{A=p+1}^{n}(y^A)^2\ , \tag{30}$$

where g_a does not depend on y.

Proof. For any O^2 function G such that $G(0)=0$,

$$G(y)=\int_0^1\frac{dG(sy)}{ds}ds=\int_0^1\frac{\partial G(sy)}{\partial(sy^\alpha)}y^\alpha ds=y^\alpha g_\alpha(y)$$

with

$$g_\alpha(y)\equiv\int_0^1\frac{\partial G(sy)}{\partial(sy^\alpha)}ds,\quad g_\alpha(0)=\frac{\partial G}{\partial(sy^\alpha)}(0)\ .$$

$g_\alpha(0)$ vanishes by virtue of (27) and (28). But, according to (27a), $\partial G/\partial y^a$ is independent of $\{y^\alpha:\alpha=1,\ldots,n\}$, otherwise we would be back in case (1), Eq. (24); hence G is linear in y^a; that is, g_a does not depend on $\{y^\alpha\}$ and g_A depends only on $\{y^A:A=l+1,\ldots,n\}$. We can, for y in the subspace of M parametrized by $\{y^A\}$, repeat for g_A the argument made for G:

$$g_A(y)=y^B h_{AB}(y)\ \text{for}\ h_{AB}(y)=\int_0^1\frac{\partial g_A}{\partial y^B}(sy)ds$$

and

$$h_{AB}(0)=\frac{1}{2}\frac{\partial^2 G}{\partial y^A\partial y^B}(0)=\frac{1}{2}\frac{\partial^2\bar{F}(\bar{x}_0)}{\partial\bar{x}_0^A\partial\bar{x}_0^B}\ ,\ \det h_{AB}(0)\neq 0\ .$$

Hence

$$G(y)=\sum_{a=1}^{l}y^a g_a+\sum_{A=l+1}^{n}y^A y^B h_{AB}(y^{l+1},\ldots,y^n)\ . \tag{31}$$

y is a nondegenerate critical point in the subspace of M parametrized by $\{y^A\}$; the diagonalization of $\sum y^A y^B h_{AB}$ can be done as usual[11] and (31) is brought into the form (30). Q.E.D.

It follows from the fact that (22) can be split into (27a) and (27b) that the set of critical points, all of which are degenerate, form a submanifold. We shall call $\{y^\alpha\}$ the coordinates which bring $G(y)$ into the form (30). Then

$$I=\lim_{\hbar=0}\int_{R^n}dy\,\det_{\alpha\beta}(\partial x^\alpha/\partial y^\beta)\times\exp\left[\frac{i}{\hbar}[G(y)+S(p_b,t_b;p_a,t_a)]\right]\times A(x(y))\ . \tag{32}$$

Set $y^\alpha=\hbar u^\alpha$ and $\det(\partial x^\alpha/\partial y^\beta)A(x(y))=D(y)$. Then

$$I=\lim_{\hbar=0}\exp\left[\frac{i}{\hbar}S(p_b,t_b;p_a,t_a)\right]\hbar^n\times\int_{R^n}du\,\exp\left[\frac{i}{\hbar}G(\hbar u)\right][D(0)+O(\hbar)] \tag{33}$$

with

$$\hbar^{-1}G(\hbar u)=\sum_{a=1}^{l}u^a g_a+\tfrac{1}{2}\hbar\sum_{A=l+1}^{n}(\pm)(u^A)^2\ .$$

In the limit $\hbar=0$, the integrations over $u^1,\ldots,u^l$ contribute a factor $(2\pi)^l\delta(g_1)\cdots\delta(g_l)$; the integrations over $\hbar u^{l+1}=y^{l+1},\ldots,\hbar u^n=y^l$ can be done by the stationary-phase approximation. It remains to compute

$$D(0)\equiv\det_{\alpha\beta}(\partial x^\alpha/\partial y^\beta)A(x(y)) \text{ at } y=0\ . \tag{34}$$

The change of variables $\{x^\alpha\}$ into $\{\bar{x}^\alpha\}$ into $\{y^\alpha\}$ diagonalizes the Hessian of G,

$$\frac{\partial^2F}{\partial x^\alpha\partial x^\beta}\frac{\partial x^\alpha}{\partial y^\delta}\frac{\partial x^\beta}{\partial y^\gamma}=\frac{\partial^2G}{\partial y^\delta\partial y^\gamma}$$

$$=\left|\begin{matrix}\left.\begin{matrix}0 & & \\ & \ddots & \\ & & 0\end{matrix}\right\}l & & \\ & \left.\begin{matrix}-1 & & \\ & \ddots & \\ & & -1\end{matrix}\right\}p & \\ & & \left.\begin{matrix}1 & & \\ & \ddots & \\ & & 1\end{matrix}\right\}q\end{matrix}\right|. \tag{35}$$

Let $N^\beta{}_\gamma(t_a,t)$ be the matrix inverse of $K^\alpha{}_\beta(t,t_a)=\partial q^\alpha(t)/\partial q^\beta(t_a)$ and let $L^\alpha{}_\beta(t,t_a)=\partial\dot{q}^\alpha(t)/\partial q^\beta(t_a)$ for q defined by $(p_a,t_a)(p_b,t_b)$ [see Eq. (43), the calculation of $D(0)$ carried out in terms of ϵ limits rather than schematically as in (38)]. Equation (35) can be rewritten as follows, with $D(0)$ given by (34) and (21) and T_a and T_b set temporarily equal to 1,

$$[(\det_{\alpha\beta}\tilde{N}_\alpha{}^\beta(t,t_b)]^{-1}\det_{\alpha\beta}\partial^2F/\partial x^\alpha\partial x^\beta[\det_{\alpha\beta}N^\alpha{}_\beta(t_a,t)]^{-1}D^2 =0^l(-1)^p(1)^q\ . \tag{36}$$

On the other hand, by virtue of (A30), (A35), and (A65),

$$\begin{aligned}\partial^2F/\partial x^\alpha\partial x^\beta&=[L(t,t_a)N(t_a,t)-L(t,t_b)N(t_b,t)]_{\alpha\beta}\\&=[\tilde{N}(t,t_b)L(t_b,t_a)N(t_a,t)]_{\alpha\beta}\ .\end{aligned} \tag{37}$$

Inserting this expression for $\partial^2F/\partial x^\alpha\partial x^\beta$ into (36) gives [see Appendix A, particularly (A6), (A8), (A15b), (A30), (A35), and (A65)]

$$\begin{gathered}\det_{\alpha\beta}L_{\alpha\beta}(t_b,t_a)[D(0)]^2=0^l(-1)^p(1)^q\ ,\\ \left|0^l\prod_{A=l+1}^{n}\lambda_{(A)}\right|[D(0)]^2=|0^l(-1)^p(1)^q|\ ,\end{gathered} \tag{38}$$

where $\lambda_{(A)}$ are the nonzero eigenvalues of $L_{\alpha\beta}$. Finally, for T_a and T_b not necessarily constant mappings,

$$I=(2\pi\hbar)^{(n-l)/2}\exp[(q-p)i\pi/4]\exp\left[\frac{i}{\hbar}S(p_b,t_b;p_a,t_a)\right]\left[\prod_{A=l+1}^{n}\lambda_{(A)}\right]^{-1/2}T_a(q(t_a))T_b(q(t_b))(2\pi\hbar)^l\delta(g_1)\cdots\delta(g_l)\ . \tag{39}$$

Set

$$\hat{\mathcal{K}}_{\text{WKB}}(p_b,t_b;p_a,t_a)=(2\pi\hbar)^{(n-l)/2}\exp[(q-p)i\pi/4]\exp\left[\frac{i}{\hbar}S(p_b,t_b;p_a,t_a)\right]\left[\prod_{A=l+1}^{n}\lambda_{(A)}\right]^{-1/2}T_a(q(t_a))T_b(q(t_b))\ . \tag{40}$$

In conclusion,

$$\mathcal{K}_{\text{WKB}}(p_b,t_b;p_a,t_a)=\hat{\mathcal{K}}_{\text{WKB}}(p_b,t_b;p_a,t_a)(2\pi\hbar)^l\delta(g_1)\cdots\delta(g_l)\ , \tag{41}$$

where the set $\{g_a=0{:}a=1,\ldots,l\}$ is the set of conservation laws (27a).

III. EXAMPLES

A. Free particle

This is an example where the initial and final wave functions are not of compact support and Eq. (24) is not valid. The WKB approximation is exact,

$$\begin{aligned}\mathcal{K}(p_b,t_b;x,t)&=\exp\left[\frac{i}{\hbar}\left[\int_t^{t_b}\tfrac{1}{2}|p_b|^2dt-p_{b\alpha}[x+p_b(t_b-t)]^\alpha\right]\right]\\&=\exp\left[\frac{i}{\hbar}[-\tfrac{1}{2}|p_b|^2(t_b-t)-p_{b\alpha}x^\alpha]\right],\end{aligned}$$

$$\mathcal{K}(x,t;p_a,t_a)=\exp\left[\frac{i}{\hbar}[-\tfrac{1}{2}|p_a|^2(t-t_a)+p_{a\alpha}x^\alpha]\right]\ ,$$

and

$$\mathcal{K}(p_b,t_b;p_a,t_a)=(2\pi\hbar)^3\delta(p_a-p_b)\exp\left[-\frac{i}{2\hbar}|p_a|^2(t_b-t_a)\right]\ . \tag{42}$$

B. Scattering by a central field

Consider a particle of mass m in a spherically-symmetric potential $V(r)$. The choice of the initial and final wave functions ϕ_a and ϕ_b is dictated by the transition we are interested in. For instance, we may want the momentum-to-momentum transition amplitude $\mathcal{K}(p_b,t_b;p_a,t_a)$ characterized by the vectors p_a and p_b, or we may want the angular momentum-to-angular momentum-transition amplitude

$$\mathcal{K}(p_{rb},p_{\theta b},p_{\phi b},t_b;p_{ra},p_{\theta a},p_{\phi a},t_a)\ ,$$

or we may want a momentum-to-angular momentum transition, or vice versa. In the first case, the flows have to be made of parallel paths in the distant past and future. In the second case, the flows have to be made of radial paths in the distant past and future (see Figs. 3 and 4). Indeed, "given p_a" means "given an incident plane." "Given $p_{ra},p_{\theta a},p_{\phi a}$" means "given an incident spherical wave," since the radial paths have constant $p_{\theta a}$ and constant $p_{\phi a}$;

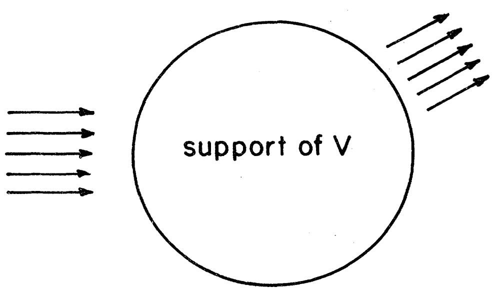

FIG. 3. Incoming and outgoing flows corresponding to a momentum-to-momentum transition $\mathscr{K}(p_b,t_b;p_a,t_a)$.

in the distant past $|p_a| = |p_{ar}| = (2mE_a)^{1/2}$.

Note first that for t_a and t_b sufficiently large one can characterize the classical path q either by

$$(p_a,t_a)(p_b,t_b)$$

or by

$$(p_{ra},p_{\theta a},p_{\phi a},t_a)(p_{rb},p_{\theta b},p_{\phi b},t_b)$$

and the corresponding action functions are the same: The contributions from the Lagrangian are obviously the same, the contributions from the boundary terms are the same because

$$p_{a\alpha}q^{\alpha}(t_b)=\frac{m}{2}d\,|q(t)|^2/dt\,|_{t=t_b}$$
$$=\frac{m}{2}dr^2(t)/dt\,|_{t=t_b}$$
$$=p_{ar}r(t_b)=(2mE_a)^{1/2}r(t_b)\ .$$

(i) Momentum-to-momentum transition $\mathscr{K}(p_b,t_b;\ p_a,t_a)$. To compare (40) with the classical results we shall use cylindrical coordinates at t_a,

$$\{a^i\}=\{z,b,\varphi\}$$

and polar coordinates at t_b in momentum space:

$$\{p_{bi}\}=\{\,|p_b|,\theta,\Phi\}\ .$$

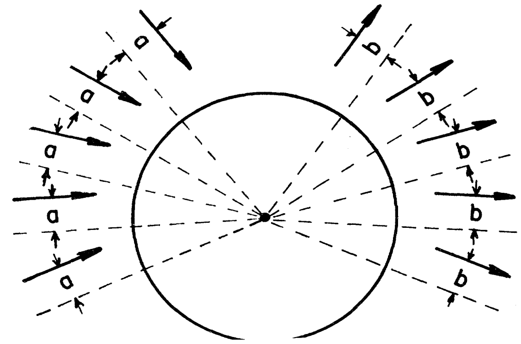

FIG. 4. Incoming and outgoing flows corresponding to an angular-momentum-to-angular-momentum transition $\mathscr{K}(p_{rb},p_{\theta b},p_{\phi b},t_b;\ p_{ra},p_{\theta a},p_{\phi a},t_a)$.

Then the bivector $L_{\alpha\beta}(t_b,t_a)=\partial p_{b\alpha}/\partial a^{\beta}$ in Cartesian coordinates can be written

$$L_{\alpha\beta}(t_b,t_a)=\frac{\partial p_{b\alpha}}{\partial p_{bi}}\frac{\partial p_{bi}}{\partial a^j}\frac{\partial a^j}{\partial a^{\beta}}$$

with

$$\det_{\alpha i}\partial p_{b\alpha}/\partial p_{bi}=|p_b|^2\sin\theta,$$
$$\det_{j\beta}\partial a^j/\partial a^{\beta}=b^{-1}\ ,$$

and

$$\frac{\partial p_{bi}}{\partial a^j}=\begin{bmatrix}\epsilon & \epsilon & \epsilon\\ \epsilon & d\theta/\partial b & 0\\ 0 & 0 & 1\end{bmatrix}, \tag{43}$$

where $\epsilon\to 0$ when $t_b\to\infty$. On the other hand (38),

$$\det L_{\alpha\beta}(t_b,t_a)D^2=\det\begin{bmatrix}\epsilon & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 1\end{bmatrix}=\epsilon\ .$$

Thus

$$[D(0)]^2=\epsilon/\epsilon\,|p_b|^2\sin\theta b^{-1}(\partial\theta/\partial b)$$
$$=b(\,|p_b|^2\sin\theta\,\partial\theta/\partial b)^{-1}$$

and

$$\mathscr{K}_{\mathrm{WKB}}(p_b,t_b;p_a,t_a)=(2\pi\hbar)\exp\left[\frac{i\pi}{2}\right]\exp\left[\frac{i}{\hbar}S(p_b,t_b;p_a,t_a)\right]\frac{b^{1/2}}{|p_b|}\left[\sin\theta\frac{\partial\theta}{\partial b}\right]^{-1/2}T_a(q(t_a))T_b(q(t_b))2\pi\hbar\delta(\,|p_b|-|p_a|\,)\ . \tag{44}$$

The conservation law can be read off the first row of $\partial p_{bi}/\partial a^j$ (namely, $|p_b|$ does not depend on the initial position of the particle, provided t_a and t_b are large enough).

(ii) Angular-momentum-to-angular-momentum transition, $\mathscr{K}(p_{rb},p_{\theta b},p_{\varphi b},t_b;p_{ra},p_{\theta a},p_{\varphi a},t_a)$.

If, in (20), we change coordinates from Cartesian $\{x^{\alpha}\}$ to polar $\{\bar{x}^{\alpha}\}=\{r,\theta,\varphi\}$, we change the state representation from momentum $\{p_{\alpha}\}$ to angular momentum $\{p_r,p_{\theta},p_{\varphi}\}$. In polar coordinates,

$$\bar{F}(\bar{x})=\int_r^{r_b}p_{br}dr_b+\int_{\theta}^{\theta_b}p_{b\theta}d\theta_b+\int_{\varphi}^{\varphi_b}p_{b\varphi}d\varphi_b-p_{br}r_b(t_b)-\int_t^{t_b}E_b dt$$
$$+\int_{r_a}^{r}p_{ar}dr_a+\int_{\theta_a}^{\theta}p_{a\theta}d\theta_a+\int_{\varphi_a}^{\varphi}p_{a\varphi}d\varphi_a+p_{ar}r_a(t_a)-\int_{t_a}^{t}E_a dt\ . \tag{45}$$

The change from Cartesian to polar coordinates does not fully bring the Hessian of F in the form (35). But it is not necessary to do so.

(a) It is clear that $\bar{F}_{,\theta}=0$ and $\bar{F}_{,\varphi}=0$ are conservation laws. (b) $\bar{F}_{,r}=0$ says $p_{br}(r)=p_{ar}(r)$; it does not determine r other than saying r is on the classical path defined by the initial conditions at t_a and the final conditions at t_b. p_r is not a constant of the motion but an asymptotic constant of the motion, $p_r(t_b)=p_r(t_a)$ for t_a and t_b sufficiently large. $\bar{F}_{,rr}=0$ at any r which makes $\bar{F}_{,r}=0$. All the eigenvalues of $L_{\alpha\beta}(t_b,t_a)$ are either zero or vanishing in the remote past and future. Thus

$$\mathscr{K}_{\mathrm{WKB}}(p_{rb},p_{\theta b},p_{\varphi b},t_b;p_{ra},p_{\theta a},p_{\varphi a},t_a)=\exp(3i\pi/4)\exp\left[\frac{i}{\hbar}S(p_{rb},p_{\theta b},p_{\varphi b},t_b;p_{ra},p_{\theta a},p_{\varphi a},t_a)\right]T_a(q(t_a)T_b(q(t_b))$$
$$\times(2\pi\hbar)^3\delta(p_{rb}-p_{ra})\delta(p_{\theta b}-p_{\theta a})\delta(p_{\varphi b}-p_{\varphi a})\ . \tag{46}$$

Equations (44) and (46) can be compared with the classical equations obtained via angular decomposition (partial-wave decomposition). For instance, the δ functions in (44) are the same as the δ functions in the equation derived by Mott and Massey[12] [their equations (66) and (57), pp. 97—102] and the δ functions in (46) can be obtained, in the limit $t_a=-\infty$, $t_b=\infty$, from the δ functions in the equation derived by Schiff[13] (his pages 322—323) for

$$\mathscr{K}_{\mathrm{WKB}}(\,|p_b|,L_b,M_b,\infty;|p_a|,L_a,M_a,-\infty)\ .$$

Since the Mott and Massey, and the Schiff formulas are valid for $t_a=-\infty$ and $t_b=+\infty$, we postpone the comparison of the WKB scattering amplitudes obtained via path integration and via the Schrödinger formalism to the third paper[5] which deals with these limits.

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APPENDIX: JACOBI FIELDS AND WKB APPROXIMATIONS

A self-contained supplement to "Jacobi fields and related topics"[14] leading to WKB approximations for different boundary conditions is presented in this appendix.

(1) The Jacobi fields. Let

$$\underline{S}(q,t_b,t_a)\equiv\int_{t_a}^{t_b}L(q(t),\dot{q}(t))dt$$

be the action of a system S, and let its configuration space be a Riemannian manifold M with metric tensor $g_{\mu\nu}=\partial^2L/\partial\dot{q}^\mu\partial\dot{q}^\mu$; we use $\|\ \|$ for the corresponding norm and $|\ |$ for the Euclidean norm.[15] Thus if

$$L=\frac{m}{2}|\dot{q}|^2-V(q)\ ,$$

then $\|q\|^2=m|\dot{q}|^2$ and $\|p\|^2=|p|^2/m$.

The Jacobi operator $\mathscr{J}(q)$ along a classical path q of the system is

$$\mathscr{J}(q)=-L_{22}\frac{d^2}{dt^2}+\left[L_{12}-L_{21}-\frac{dL_{22}}{dt}\right]\frac{d}{dt}+\left[L_{11}-\frac{dL_{21}}{dt}\right]\ , \tag{A1}$$

where L_1 and L_2 are the derivatives of L with respect to its first and second arguments, respectively, and L_{11}, L_{12}, L_{21}, and L_{22} are defined similarly; for example, $(L_{21})_{\mu\nu}=\partial^2L/\partial\dot{q}^\mu\partial q^\nu$.

The Jacobi fields are the solutions of the Jacobi equation (also called the small disturbance equation, or the equation of geodetic deviation in the context of Riemannian geometry):

$$\mathscr{J}(q)h(t)=0\ . \tag{A2}$$

This equation has, in general, $2n$ linearly independent solutions. Each one can be obtained through a one-parameter variation through classical paths.

Let $\{q(t,\alpha)\}$, with α a $2n$ index, be the family of classical paths. For instance, α could be the $2n$ constants of integration of the Euler-Lagrange equations. The $2n$ one-parameter variations $\{\partial q(t,\alpha)/\partial\alpha_i : i=1\cdots 2n\}$ define $2n$ Jacobi fields. Note that the velocity field $\partial q(t,\alpha)/\partial t$ is also a Jacobi field if L has no explicit time dependence; it can be expressed as a linear combination[16] of $\{\partial q(t,\alpha)/\partial a_i\}$.

In the case of a velocity-dependent potential we shall set

$$V(q(t),\dot{q}(t))=\mathscr{V}(q(t))+\langle A(q(t)),\dot{q}(t)\rangle \quad \text{for } A(q(t))\in T^*_{q(t)}M\ . \tag{A3}$$

The terms quadratic in $\dot{q}$ contribute to the kinetic energy. Velocity-dependent potentials have been investigated by Nelson and Sheeks.[2]

(2) The small disturbance of the small disturbances. If we take the derivatives with respect to α_i or to t of the Jacobi equations

$$\mathscr{J}(q(\alpha))\partial q(t,\alpha)/\partial\alpha_i=0$$

or

$$\mathscr{J}(q(\alpha))\partial q(t,\alpha)/\partial t=0\ ,$$

we obtain the equations satisfied by the variations of the Jacobi fields. For instance, if $L(q,\dot{q})=\frac{1}{2}m\|\dot{q}\|^2-V(q)$, then

$$\mathscr{I}_{\mu\nu}\frac{\partial^2 q^\nu}{\partial\alpha_i\partial\alpha_j}=\frac{\partial q^\nu}{\partial\alpha_i}\frac{\partial q^\rho}{\partial\alpha_j}\nabla_\mu\nabla_\nu\nabla_\rho V(q) ,$$
$$\mathscr{I}_{\mu\nu}\frac{\partial^2 q^\nu}{\partial\alpha_i\partial t}=\frac{\partial q^\nu}{\partial\alpha_i}\frac{\partial q^\rho}{\partial t}\nabla_\mu\nabla_\nu\nabla_\rho V(q) , \quad \text{(A4)}$$
$$\mathscr{I}_{\mu\nu}\frac{\partial^2 q^\nu}{\partial t^2}=\frac{\partial q^\nu}{\partial t}\frac{\partial q^\rho}{\partial t}\nabla_\mu\nabla_\nu\nabla_\rho V(q) .$$

These equations can be solved with the Green's functions of the Jacobi equation which has the appropriate boundary conditions.

(3) The Jacobi matrices.

$J^\mu{}_\nu(t,t_a)$ and $K^\mu{}_\nu(t,t_a)$ are bivectors defined as follows. $J(t,t_a)$ and $K(t,t_a)$ are mappings from $T_{q(t_a)}M$ into $T_{q(t)}M$ such that, for $v\in T_{q(t_a)}M$,

$$J^\mu{}_\nu(t,t_a)v^\nu=j^\mu(t) , \quad \text{(A5)}$$

where j is a Jacobi field along q with Cauchy data $j^\mu(t_a)=0, \dot{j}^\mu(t_a)=v^\mu$;

$$K^\mu{}_\nu(t,t_a)v^\nu=k^\mu(t) , \quad \text{(A6)}$$

where k is a Jacobi field along q with Cauchy data[17] $k^\mu(t_a)=v^\mu$,

$$\dot{k}^\mu(t_a)=\tfrac{1}{2}g^{\mu\nu}\{A_{\nu,\rho}[q(t_a)]-A_{\rho,\nu}[q(t_a)]\}v^\rho ,$$

where A is defined by (A3). Note that $\dot{k}^\mu(t_a)=0$ for velocity-independent potentials.

Each column of $J^\mu{}_\nu(t,t_a)$ consists of the components $j^\mu{}_{(\nu)}$ of the n Jacobi field $\{j_{(\nu)}\}$ with the boundary conditions $j^\mu{}_{(\nu)}(t_a)=0$, and $\dot{j}^\mu{}_{(\nu)}(t_a)=\delta^\mu{}_\nu$.

Each column of $K^\mu{}_\nu(t,t_a)$ consists of the components $k^\mu{}_{(\nu)}$ of the n Jacobi field $\{k_{(\nu)}\}$ with the boundary conditions $k^\mu{}_{(\nu)}(t_a)=\delta^\mu{}_\nu$, and $\dot{k}^\mu{}_{(\nu)}(t_a)=0$ for velocity-independent potentials.

If we specify a classical path $q(t,a,v_a)$ by its initial position $q(t_a,a,v_a)=a$ and its initial velocity $\dot{q}(t_a,a,v_a)=v_a$, then

$$J^\mu{}_\nu(t,t_a)=\partial q^\mu(t,a,v_a)/\partial v_a{}^\nu , \quad \text{(A7)}$$

$$K^\mu{}_\nu(t,t_a)=\partial q^\mu(t,a,v_a)/\partial a^\nu . \quad \text{(A8)}$$

Note[18] that

$$J^{\mu\nu}(t,s)=\frac{\partial q^\mu(t,a,v_a)}{\partial p_{a\rho}}\frac{\partial q^\nu(s,a,v_a)}{\partial a^\rho}-\frac{\partial q^\mu(t,a,v_a)}{\partial a^\rho}\frac{\partial q^\nu(s,a,v_a)}{\partial p_{a\rho}} , \quad \text{(A9)}$$

so that $J(t,s)$ is the commutator function. Also,

$$K^\mu{}_\nu(t,s)=\frac{\partial q^\mu(t,a,v_a)}{\partial a^\rho}\frac{\partial p_\nu(s,a,v_a)}{\partial p_{a\rho}}-\frac{\partial q^\mu(t,a,v_a)}{\partial p_{a\rho}}\frac{\partial p_\nu(s,a,v_a)}{\partial a^\rho} . \quad \text{(A10)}$$

It can be proved[19] that $\widetilde{K}(t,t_a)$ defined by $\widetilde{K}^\mu{}_\nu(t,t_a)\equiv K_\nu{}^\mu(t_a,t)$ satisfies

$$\widetilde{K}^\mu{}_\nu(t,t_a)=\nabla_t J^\mu{}_\nu(t,t_a)=\partial\dot{q}^\mu(t,a,v_a)/\partial v^\nu{}_a . \quad \text{(A11)}$$

It is convenient also to introduce

$$L^\mu{}_\nu(t,t_a)\equiv\nabla_t K^\mu{}_\nu(t,t_a)=\partial\dot{q}^\mu(t,a,v_a)/\partial a^\nu , \quad \text{(A12)}$$

$\widetilde{K}(t,t_a)$ and $L(t,t_a)$ are solutions of the small disturbances of the small disturbances of (A4). Note that L can be written as

$$L_{\mu\nu}(t,s)=\frac{\partial p_\mu(t,a,v_a)}{\partial a^\rho}\frac{\partial p_\nu(s,a,v_a)}{\partial p_{a\rho}}-\frac{\partial p_\mu(t,a,v_a)}{\partial p_{a\rho}}\frac{\partial p_\nu(s,a,v_a)}{\partial a^\rho} .$$

The symmetry properties of J,K,L are the following:

(i) $J(t,s)=-\widetilde{J}(t,s)$, i.e., $J^{\alpha\beta}(t,s)=-J^{\beta\alpha}(s,t)$. *Proof:* In subsection (4) of this appendix, we prove the antisymmetry property of its "inverse." (A13)

(ii) In general, K has no symmetry property.

(iii) $L(t,s)=-\widetilde{L}(t,s)$, i.e., $L^{\alpha\beta}(t,s)=-L^{\beta\alpha}(s,t)$. *Proof:* Follows from the definition, together with (A11). (A14)

$J,\widetilde{K},K,L$ make a matrix which is the solution of the Jacobi operator in phase space.[20] Let H be the Hamiltonian, then

$$\begin{bmatrix}\partial^2H/\partial q^\alpha\partial q^\beta & -\delta^\beta_\alpha\partial/\partial t-\partial^2H/\partial q^\alpha\partial p_\beta\\ \delta^\alpha_\beta\partial/\partial t-\partial^2H/\partial p_\alpha\partial q^\beta & -\partial^2H/\partial p_\alpha\partial p_\beta\end{bmatrix}\begin{bmatrix}J^{\alpha\gamma}(t,s) & K^\alpha{}_\gamma(t,s)\\ \widetilde{K}_\alpha{}^\gamma(t,s) & L_{\alpha\gamma}(t,s)\end{bmatrix}=0 .$$

(4) J, K, and L are bivectors. It is sometimes convenient to treat them as matrices. Their "inverses" M, N, and P, defined by

$$M^\mu{}_\nu(t_a,t)J^\nu{}_\rho(t,t_a)=\delta^\mu_\rho , \quad \text{(A15a)}$$

$$N^\mu{}_\nu(t_a,t)K^\nu{}_\rho(t,t_a)=\delta^\mu_\rho , \quad \text{(A15b)}$$

$$P^\mu{}_\nu(t_a,t)L^\nu{}_\rho(t,t_a)=\delta^\mu_\rho , \quad \text{(A15c)}$$

are the Van Vleck determinants corresponding to the various action functions.

Proof: Let $\{\bar{q}(\alpha)\}$ be a one-parameter variation through classical paths

$$\bar{q}(\alpha)(t)\equiv q(t,\alpha) . \quad \text{(A16)}$$

Let the boundary values of $\bar{q}(0)$ be

$$q(t_a,0)=a \ , \ \dot{q}^\beta(t_a,0)=p^\beta_a ,$$

$$q(t_b,0)=b \ , \ \dot{q}^\beta(t_b,0)=p^\beta_b .$$

The action functions S corresponding to the different boundary conditions chosen to define $\bar{q}(\alpha)$ are, respectively,

$$S(q(t_b,\alpha),q(t_a,\alpha))=\underline{S}(\bar{q}(\alpha),t_b,t_a) \quad \text{for } \bar{q}(\alpha) \text{ defined by the initial position, final position,} \tag{A17a}$$

$$S(q(t_b,\alpha),\dot{q}(t_a,\alpha))-S_a(q(t_a,\alpha),\dot{q}(t_a,\alpha)) =\underline{S}(\bar{q}(\alpha),t_b,t_a) \quad \text{for } \bar{q}(\alpha) \text{ defined by the initial momentum, final position,} \tag{A17b}$$

$$S(\dot{q}(t_b,\alpha),q(t_a,\alpha))+S_b(q(t_b,\alpha),\dot{q}(t_b,\alpha)) =\underline{S}(\bar{q}(\alpha),t_b,t_a) \quad \text{for } \bar{q}(\alpha) \text{ defined by the initial position, final momentum,} \tag{A17c}$$

and

$$S(\dot{q}(t_b,\alpha),\dot{q}(t_a,\alpha))+S_b(q(t_b,\alpha),\dot{q}(t_b,\alpha)) -S_a(q(t_a,\alpha),\dot{q}(t_a,\alpha)) =\underline{S}(\bar{q}(\alpha),t_b,t_a) \quad \text{for } \bar{q}(\alpha) \text{ defined by initial momentum, final momentum .} \tag{A17d}$$

The end-point contributions are such that both sides of these equations vanish when $t_b=t_a$. We can take

$$S_a(q(t_a,\alpha),\dot{q}(t_a,\alpha))=\dot{q}_\alpha(t_a,\alpha)q^\alpha(t_a,\alpha) =\tfrac{1}{2}d\,|\,q(t_a)\,|^2/dt_a \tag{A18a}$$

and

$$S_b(q(t_b,\alpha),\dot{q}(t_b,\alpha))=\tfrac{1}{2}d\,|\,q(t_b)\,|^2/dt_b \ . \tag{A18b}$$

To prove that the inverses M,N,P defined by (A15) are Van Vleck matrices, we expand both sides of (A17) in powers of α. Since $\{\bar{q}(\alpha)\}_\alpha$ is a variation through classical paths, the expansion of the right-hand side gives

$$\underline{S}(\bar{q}(\alpha))=\underline{S}(\bar{q}(0)) +\alpha L_2 h(t)\Big|_{t_a}^{t_b}+\tfrac{1}{2}\alpha^2\left[L_{21}-\frac{1}{2}\frac{d}{dt}L_{22}\right]h(t)h(t)\Big|_{t_a}^{t_b} +\tfrac{1}{4}\alpha^2\frac{d}{dt}[L_{22}h(t)h(t)]\Big|_{t_a}^{t_b}+\tfrac{1}{2}\alpha^2 L_2\partial^2 q(t,\alpha)/\partial\alpha^2\Big|_{t_a}^{t_b}+\cdots \ , \tag{A19}$$

where $h(t)\equiv\partial\bar{q}(\alpha,t)/\partial\alpha\,|_{\alpha=0}$ is a Jacobi field along $\bar{q}(0)$. For

$$L(q,\dot{q})=\tfrac{1}{2}||\dot{q}||^2-V(q) \ , \tag{A20}$$

$$\underline{S}(\bar{q}(\alpha))=\underline{S}(\bar{q}(0))+\alpha L_2 h(t)\Big|_{t_a}^{t_b}+\alpha^2(\dot{h}(t)\,|\,h(t))\Big|_{t_a}^{t_b}+\tfrac{1}{2}\alpha^2 L_2\frac{\partial^2 q(t,\alpha)}{\partial\alpha^2}\Big|_{t_a}^{t_b}+\cdots \ . \tag{A21}$$

The zero-order terms of the expansion of (A17) give the relations between the various action functions S and the action functional $\underline{S}$.

(i) For $\bar{q}(\alpha)$ defined by initial position, final position, the terms of order α give

$$\frac{\partial S}{\partial b}(b,t_b;a,t_a)h(t_b)+\frac{\partial S}{\partial a}(b,t_b;a,t_a)h(t_a)=p_b h(t_b)-p_a h(t_a) \ , \tag{A22}$$

which shows that the action function is the generating function of a canonical transformation, namely the time-dependent point transformation where the a's are the old variables, and the b's are the new ones.

To compare the terms of order α^2, we need to express $\dot{h}(t_a)$ and $\dot{h}(t_b)$ in terms of $h(t_a)$ and $h(t_b)$ in (A19):

$$\begin{aligned} h(t)&=J(t,t_a)M(t_a,t_b)h(t_b)+J(t,t_b)M(t_b,t_a)h(t_a) \ , \\ \dot{h}(t)&=\tilde{K}(t,t_a)M(t_a,t_b)h(t_b)+\tilde{K}(t,t_b)M(t_b,t_a)h(t_a) \ , \end{aligned} \tag{A23}$$

$$\begin{aligned} (\dot{h}(t_b)\,|\,h(t_b))&=(\tilde{K}(t_b,t_a)M(t_a,t_b)h(t_b)\,|\,h(t_b))+(M(t_b,t_a)h(t_a)\,|\,h(t_b)) \ , \\ (\dot{h}(t_a)\,|\,h(t_a))&=(M(t_a,t_b)h(t_b)\,|\,h(t_a))+(\tilde{K}(t_a,t_b)M(t_b,t_a)h(t_a)\,|\,h(t_a)) \ . \end{aligned} \tag{A24}$$

Equating the cross terms $h(t_a)h(t_b)$ on both sides of (A17a) gives

$$\partial^2 S(b,t_b;a,t_a)/\partial b^\beta\partial a^\alpha=M_{\beta\alpha}(t_b,t_a) =-M_{\alpha\beta}(t_a,t_b) \ . \tag{A25}$$

For systems with constant metric tensor and velocity-independent potentials (A20),

$$\partial^2 S(b,t_b;a,t_a)/\partial b^\beta\partial b^\alpha=\tilde{K}_\beta{}^\gamma(t_b,t_a)M_{\gamma\alpha}(t_a,t_b) \tag{A26}$$

and

$$\partial^2 S(b,t_b;a,t_a)/\partial a^\beta\partial a^\alpha=-\tilde{K}_\beta{}^\gamma(t_a,t_b)M_{\gamma\alpha}(t_b,t_a) \ . \tag{A27}$$

For arbitrary systems, one uses the Jacobi matrix K satisfying the boundary conditions given by Nelson and Sheeks[2] and one proceeds as before using the full expression (A19) rather than the simplified equation (A21).

(ii) For $\bar{q}(\alpha)$ defined by initial momentum, final position, the terms of order α in the expansion of (A17b) give

$$\frac{\partial S}{\partial b}h(t_b)+\left[\frac{\partial S}{\partial p_a}\,\Big|\dot h(t_a)\right]-\frac{\partial S_a}{\partial a}h(t_a)-\left[\frac{\partial S_a}{\partial p_a}\,\Big|\dot h(t_a)\right]=p_b h(t_b)-p_a h(t_a)\;.$$

Here, the inner product $(\,|\,)$ is defined with the metric $g_{\alpha\beta}\equiv\partial^2 h/\partial\dot q^\alpha\partial\dot q^\beta$; and juxtaposition implies a contraction, e.g., $(\partial S/\partial b)h\equiv(\partial S/\partial b^\alpha)h^\alpha$. The argument of S_a is (a,p_a), where $a=\Phi^{-1}_{t_b-t_a}(b)$ with Φ the classical flow defined by (15):

$$\frac{\partial S}{\partial p_a}(b,t_b;p_a,t_a)=\frac{\partial S_a}{\partial p_a}(a,p_a)\;, \tag{A28a}$$

$$\frac{\partial S}{\partial b}(b,t_b;p_a,t_a)=p_b\;, \tag{A28b}$$

$$\frac{\partial S_a}{\partial a}(a,p_a)=p_a\;. \tag{A28c}$$

If $S_a(a,p_a)=a^\alpha p_{a\alpha}$, then

$$\frac{\partial S}{\partial p_a}(b,t_b;p_a t_a)=a\;.$$

To compare the terms of order α^2, we need to express $h(t_a)$ and $\dot h(t_b)$ in terms of $\dot h(t_a)$ and $h(t_b)$:

$$h(t)=K(t,t_a)N(t_a,t_b)h(t_b)+J(t,t_b)\tilde N(t_b,t_a)\dot h(t_a)\;,$$

$$\dot h(t)=L(t,t_a)N(t_a,t_b)h(t_b)+K(t,t_b)\tilde N(t_b,t_a)\dot h(t_a)\;,$$

$$(\dot h(t_b)\,|\,h(t_b))=(L(t_b,t_a)N(t_a,t_b)h(t_b)\,|\,h(t_b))+(\tilde N(t_b,t_a)\dot h(t_a)\,|\,h(t_b))\;,$$

$$(\dot h(t_a)\,|\,h(t_a))=(\dot h(t_a)\,|\,N(t_a,t_b)h(t_b))+(\dot h(t_a)\,|\,J(t_a,t_b)\tilde N(t_b,t_a)\dot h(t_a))\;.$$

To simplify matters we shall take $S_a(a,p_a)=a^\alpha p_{a\alpha}$ and consider Lagrangians of type (A20). For the general case we refer to the papers of Nelson and Sheeks.[2] Equating the terms of order α^2 in (A17b) gives

$$\partial^2 S(b,t_b;p_a,t_a)/\partial b^\beta dp_{a\alpha}=\tilde N_\beta{}^\alpha(t_b,t_a)=N^\alpha{}_\beta(t_a,t_b)\;, \tag{A29}$$

$$\partial^2 S(b,t_b;p_a,t_a)/\partial b^\beta\partial b^\alpha=L^{\alpha\gamma}(t_b,t_a)N_\gamma{}^\beta(t_a,t_b)\;, \tag{A30}$$

$$\partial^2 S(b,t_b;p_a,t_a)/\partial p_{a\alpha}\partial p_{a\beta}=J_{\alpha\gamma}(t_a,t_b)\tilde N^\gamma{}_\beta(t_b,t_a)\;. \tag{A31}$$

The matrix inverse $\tilde N(t_b,t_a)$ of $\tilde K(t_a,t_b)$ is the Van Vleck matrix $S_{,bp_a}$. It is a bivector which in general has no symmetry property.

(iii) For $\bar q(\alpha)$ defined by initial position, final momentum, a similar analysis gives

$$\partial S(p_b,t_b;a,t_a)/\partial a^\alpha=-p_{a\alpha}\;, \tag{A32a}$$

$$\partial S(p_b,t_b;a,t_a)/\partial p_{b\alpha}=-\partial S_b(p_b,b)/\partial p_{b\alpha}\;, \tag{A32b}$$

$$\partial S_b(p_b,t_b;b,t_b)/\partial b^\alpha=p_{b\alpha}\;. \tag{A32c}$$

If we choose $S_b(p_b,b)=b^\alpha p_{b\alpha}$, then $S_{,p_b}(p_b,t_b;a,t_a)=-b$. With this choice for S_b and for Lagrangians of type (A20), a similar analysis gives

$$\partial^2 S(p_b,t_b;a,t_a)/\partial p_{b_\beta}\partial a^\alpha=-N^\beta{}_\alpha(t_b,t_a)=-\tilde N_\alpha{}^\beta(t_a,t_b)\;, \tag{A33}$$

$$\partial^2 S(p_b,t_b;a,t_a)/\partial p_{b_\beta}\partial p_{b_\alpha}=-J_{\alpha\gamma}(t_b,t_a)\tilde N^\gamma{}_\beta(t_a,t_b)\;, \tag{A34}$$

$$\partial^2 S(p_b,t_b;a,t_a)/\partial a^\beta\partial a^\alpha=-L^{\alpha\gamma}(t_a,t_b)N_\gamma{}^\beta(t_b,t_a)\;. \tag{A35}$$

The matrix inverse $-N(t_b,t_a)$ of $-K(t_b,t_a)$ is the Van Vleck matrix $\partial^2 S/\partial p_b\partial a$. It is a bivector which, in general, has no symmetry property.

(iv) For $\bar q(\alpha)$ defined by initial momentum, final momentum, a similar analysis gives

$$\partial S(p_b,t_b;p_a,t_a)/\partial p_{b\alpha}=-b^\alpha\;, \tag{A36a}$$

$$\partial S(p_b,t_b;p_a,t_a)/\partial p_{a\alpha}=a^\alpha\;, \tag{A36b}$$

and

$$\partial^2 S(p_b,t_b;p_a,t_a)/\partial p_{b\alpha}\partial p_{a\beta}=-P_{\alpha\beta}(t_b,t_a)=P_{\beta\alpha}(t_a,t_b)\;, \tag{A37}$$

$$\partial^2 S(p_b,t_b;p_a,t_a)/\partial p_{b\alpha}\partial p_{b\beta}=-K_\alpha{}^\gamma(t_b,t_a)P_{\gamma\beta}(t_a,t_b)\;, \tag{A38}$$

$$\partial^2 S(p_b,t_b;p_a,t_a)/\partial p_{a\alpha}\partial p_{a\beta}=K_\alpha{}^\gamma(t_a,t_b)P_{\gamma\beta}(t_b,t_a)\;. \tag{A39}$$

A similar analysis can be done in phase space (Ref. 1, p. 323). One introduces a two-parameter variation through classical paths $\{\bar q(\alpha),\bar p(\alpha,\beta)\}$ and expands the action function S and the action functional

$$S(\bar q(\alpha),\bar p(\alpha,\beta),t_b,t_a)=\int_{t_a}^{t_b}[p(t,\alpha,\beta)dq(t,\alpha)-H(q(t_a),p(t,\alpha,\beta))dt]$$

in powers of α and β. Equating terms of the same order in α and β give the same equations as the configuration space analysis.

(5) The Jacobi Green's functions.

The Jacobi fields can be used to construct the Green's functions $G(s,t)$ of the Jacobi operators with Dirichlet, von Neumann, and mixed boundary conditions. Since $G(s,t)=G(t,s)$, it is sufficient to check the two boundary conditions for one of the variables, say $t=t_a$ and $t=t_b$.

(i) Dirichlet boundary conditions $G(s,t_a)=0$, $G(s,t_b)=0$:

$$G(t,s)=\theta(s-t)J(t,t_a)M(t_a,t_b)J(t_b,s)-\theta(t-s)J(t,t_b)M(t_b,t_a)J(t_a,s)\;, \tag{A40}$$

where θ is the step function equal to 1 for positive arguments, 0 for negative arguments, and undefined otherwise.

(ii) Mixed boundary conditions[21] $G_+(s,t_b)=0$, $dG_+(s,t_a)/dt_a=0$:

$$G_+(t,s)=\theta(s-t)K(t,t_a)N(t_a,t_b)J(t_b,s) -\theta(t-s)J(t,t_b)\tilde{N}(t_b,t_a)\tilde{K}(t_a,s) \ . \quad \text{(A41)}$$

(iii) Mixed boundary conditions[21] $dG_-(s,t_b)/dt_b=0$, $G_-(s,t_a)=0$:

$$G_-(t,s)=\theta(s-t)J(t,t_a)\tilde{N}(t_a,t_b)\tilde{K}(t_b,s) -\theta(t-s)K(t,t_b)N(t_b,t_a)J(t_a,s) \ . \quad \text{(A42)}$$

(iv) von Neumann boundary conditions[1] $d\bar{G}(s,t_a)/dt_a=0$, $d\bar{G}(s,t_b)/dt_b=0$:

$$\bar{G}(t,s)=\theta(s-t)K(t,t_a)P(t_a,t_b)\tilde{K}(t_b,s) +\theta(t-s)K(t,t_b)\tilde{P}(t_b,t_a)\tilde{K}(t_a,s) \ . \quad \text{(A43)}$$

The proof of Eqs. (A40)–(A42) can be found in DeWitt-Morette.[14] The proof of (A43) is similar, but requires a new relationship between the Jacobi fields, namely,

$$K(t,t_a)P(t_a,t_b)\tilde{K}(t_b,s)-K(t,t_b)\tilde{P}(t_b,t_a)\tilde{K}(t_a,s)=J(t,s) \ . \quad \text{(A44)}$$

Proof of (A44). Both sides satisfy the Jacobi equation in t and s. Since both sides are antisymmetric in s and t, it is sufficient to check that the boundary conditions of both sides are equal for $t=t_a$ and $t=t_b$. The derivatives of both sides at $t=t_b$ are equal by virtue of (A11). The derivatives of both sides at $t=t_a$ are equal by virtue of $L(t,s)=-\tilde{L}(s,t)$ together with (A11). We are now in a position to prove (A43). Since $K(t,t_a)$ and $K(t,t_b)$ satisfy the Jacobi equation in t,

$$\mathscr{J}_t(q)G(t,s)=\delta(s-t)[(\dot{K}(s,t_a)P(t_a,t_b)\tilde{K}(t_b,s) -\dot{K}(s,t_b)\tilde{P}(t_b,t_a)\tilde{K}(t_a,s)] =\delta(s-t)$$

by virtue of (A44). Q.E.D.

It has been shown in Ref. 1 that the first three Green's functions can be used in the path-integral representation of position-to-position propagator, position-to-momentum propagator, and momentum-to-position propagator, respectively. Although we can postulate a path-integral representation of the momentum-to-momentum propagator in terms of the fourth Green's function, we have not yet been able to derive it from first principles.

WKB approximations for different boundary conditions. The WKB approximation of a wave function is given in terms of an action function and a Van Vleck determinant, i.e., in terms of an associated classical problem. The question is, how does one relate the boundary conditions of the associated classical problem to the given initial or final wave function, or vice versa? This question is difficult to answer when the WKB approximation is obtained in the most commonly used method, which consists in applying Schrödinger equation to an "appropriate" ansatz. But the question can be answered straightforwardly if one computes the WKB approximation of the wave function as given by a Feynman-Kac formula.[22] To simplify the presentation, we shall consider the system $L(q,\dot{q}) =\frac{1}{2}m\,|\dot{q}\,|^2-V(q)$ defined on an arbitrary Riemannian manifold. The results presented here are valid for arbitrary Lagrangians[23] which do not depend on powers of $\dot{q}$ higher than 2. Given an initial (final) wave function ϕ_a (ϕ_b) at time t_a (t_b), the path-integral representation of the wave function ψ_a (ψ_b) at time t for this Lagrangian is given by the Feynman-Kac formulas[22]

$$\psi_a(x,t)=\int_{Y_+} dw_+^W(y)\exp\left[-\frac{i}{\hbar}\int_{t_a}^{t} V(x+\mu y(s))ds\right]\phi_a(x+\mu y(t_a)) \ , \quad \text{(A45)}$$

$$\psi_b(x,t)=\int_{Y_-} dw_-^W(y)\exp\left[\frac{i}{\hbar}\int_{t}^{t_b} V(x+\mu y(s))ds\right]\phi_b^*(x+\mu y(t_b)) \ , \quad \text{(A46)}$$

where $\mu=(\hbar/m)^{1/2}$ Y_-, and Y_+ are the spaces of continuous paths vanishing, respectively, at t_a and at t_b, w_-^W, and w_+^W are the complex Wiener integrators defined by their Fourier transforms

$$(\mathscr{F}w_\mp^W)(\mu)=\exp\left[-\frac{i}{2}\int_T d\mu_\alpha(t)\int_T d\mu_\beta(s)G_\mp^{W\alpha\beta}(t,s)\right] \ , \quad \text{(A47)}$$

where

$$G_-^W(t,s)=\inf(t-t_a,s-t_a)\mathbb{1} \ , \quad G_+^W(t,s)=\inf(t_b-t,t_b-s)\mathbb{1} \ . \quad \text{(A48)}$$

The WKB approximations of (A45) and (A46) have been computed in Ref. 1 for the following choices of initial, or final wave functions:

(i) $\phi_a=\exp\left[\frac{i}{\hbar}S_a\right]T_a$ or $\phi_b=\exp\left[\frac{i}{\hbar}S_b\right]T_b$, (A49)

where S_a,S_b,T_a, and T_b are well-behaved functions on the configuration space. The support of T_a or T_b determines the localization of the system.

(ii) $\phi_a(x+\mu y(t_a))=\delta(x+\mu y(t_a)-a)$

or

$$\phi_b(x+\mu y(t_b))=\delta(x+\mu y(t_b)-b) \ . \quad \text{(A50)}$$

The methods developed in Ref. 1 can be used to compute WKB approximations of more general wave functions than (A45) and (A46) and for choices of initial or final wave functions other than (A49) and (A50). We shall not repeat these calculations here but only analyze the connection between the initial, or final, wave functions and the boundary conditions of the associated classical problem.

(i) The initial wave functions ϕ_a and ϕ_b given by (A49) generalizes plane waves. Indeed, if $S(x)=p_{a\alpha}x^\alpha$ and $T_a(x)=1$, then ϕ is the plane wave of momentum p_a. Choosing (A49) for the initial or final wave function is particularly convenient for the semiclassical approximation because, in the limit $\hbar=0$, the initial and final current densities

$$j=\hbar[\phi^*\nabla\phi-(\nabla\phi)^*\phi]/2im$$

are, respectively,

$$\lim_{\hbar=0} j_a(x)=|T(x)|^2\nabla S_a(x)/m\ ,$$
$$\lim_{\hbar=0} j_b(x)=|T_b(x)|^2\nabla S_b(x)/m\ . \tag{A51}$$

Hence, given an initial (final) wave function (A49), the associated classical problem is the classical *flow* of trajectories whose initial (final) momenta are

$$p_a(x)=\nabla S_a(x)\ ,\ \ [p_b(x)=\nabla S_b(x)]. \tag{A52}$$

If ϕ_a or ϕ_b are plane waves, the wave functions ψ_a or ψ_b are the probability amplitude for momentum-to-position transition $\mathscr{K}(x,t;p_a,t_a)$ or the probability amplitude for position-to-momentum transition $\mathscr{K}(x,t;p_b,t_b)$. We shall still use the notation $\mathscr{K}_{\rm WKB}(x,t;p_a,t_a)$ for $\psi_{a\rm WKB}(x,t)$ with ϕ_a an arbitrary initial wave function of type (A49), and use similarly the notation $\mathscr{K}_{\rm WKB}(p_b,t_b;x,t)$. But it should be remembered that when ϕ_a or ϕ_b is not a plane wave the associated classical *flow* (A52) cannot be "replaced" by an associated classical trajectory defined by $(p_a,t_a)(x,t)$ or $(x,t)(p_b,t_b)$.

If the classical flow defined by the initial or final wave function defines a one-one map in the subspace of the configuration space where the wave function is defined, then

$$\mathscr{K}_{\rm WKB}(x,t;p_a,t_a) = |\det N^\alpha{}_\beta(t_a,t)|^{1/2}\exp\left[\frac{i}{\hbar}S(x,t;p_a,t_a)\right]T_a(q(t_a))\ , \tag{A53}$$

$$\mathscr{K}_{\rm WKB}(p_b,t_b;x,t)=|\det\tilde{N}_\alpha{}^\beta(t,t_b)|^{1/2}\times\exp\left[\frac{i}{\hbar}S(p_b,t_b;x,t)\right]T_b(q(t_b))\ , \tag{A54}$$

where the action functions are given by (A17b) and (A17c) and the Van Vleck determinants are given by (A29) and (A33). It is usually easier to compute the determinant of the inverse matrix, namely, the Jacobi matrix K (A6). The case in which classical flows are caustic forming will appear in paper II (see Ref. 3, p. 3).

(ii) The wave functions given by (A45) or (A46) with the initial or final wave functions (A50) are the probability amplitudes $\mathscr{K}(x,t;a,t_a)$ that the particle known to be at a at t_a be found at x at t, and $\mathscr{K}(b,t_b;x,t)$ that the particle known to be at b at t_b was at x at t. The associated classical problems are, respectively, the associated classical flows of trajectories which originate at a, or terminate at b. They can be reduced to associated classical paths defined, respectively, by $(a,t_a)(x,t)$ or $(x,t)(b,t_b)$. If the classical flows define one-one maps in the subspace of the configuration space where the waves functions are defined, then either (A45) or (A46) gives

$$\mathscr{K}_{\rm WKB}(b,t_b;a,t_a)=(2\pi i\hbar)^{-n/2}|\det M_{\alpha\beta}(t_a,t_b)|^{1/2}\times\exp\left[\frac{i}{\hbar}S(b,t_b;a,t_a)\right]\ , \tag{A55}$$

where S is the action function (A17a) and M the Van Vleck matrix (A25). It is usually much easier to compute the determinant of the inverse matrix, namely the Jacobi matrix J (A5). The case when classical flows are caustic forming is treated in Ref. 1.

Remarks. If, in (A45), we replace $\delta(x+\mu y(t_a)-a)$ by

$$(2\pi\hbar)^{-n}\int_{\mathbb{R}^n}dp_a\exp\left[\frac{i}{\hbar}p_{a\alpha}[x+\mu y(t_a)-a]^\alpha\right]\ ,$$

then

$$\mathscr{K}(x,t;a,t_a)=(2\pi\hbar)^{-n}\int_{\mathbb{R}^n}dp_a\exp\left[-\frac{i}{\hbar}p_{a\alpha}a^\alpha\right]\times\mathscr{K}(x,t;p_a,t_a)\ , \tag{A56}$$

where $\mathscr{K}(x,t;p_a,t_a)$ is given by (A45) with ϕ_a a plane wave. Equation (A56) is the equation used in Feynman and Hibbs[24] (p. 102) to define $\mathscr{K}(x,t;p_a,t_a)$.

(7) Composition laws of the WKB approximations.

The properties of the Jacobi fields provide a proof of the composition laws of the WKB approximations. All WKB approximations are of the form

$$\mathscr{K}(\beta,t_2;\alpha,t_1)=C(\alpha,\beta)[\det\partial^2S(\beta,t_2;\alpha,t_1)/\partial\beta\partial\alpha]^{1/2}\times\exp\left[\frac{i}{\hbar}S(\beta,t_2;\alpha,t_1)\right]\ , \tag{A57}$$

where β characterizes the state of the system at time t_2 and α characterizes it at time t_1, and $C(\alpha,\beta)$ is a constant. The composition law says that, for $t_a<t<t_b$,

$$\mathscr{K}_{\rm WKB}(\gamma,t_b;\alpha,t_a) = \text{stationary-phase approximation} \times\int\mathscr{K}_{\rm WKB}(\gamma,t_b;\beta,t)\mathscr{K}_{\rm WKB}(\beta,t;\alpha,t_a)d\beta\ .$$

This is true whether or not α, β, and γ belong to the same representation. It is clear that for β a critical point

$$S(\gamma,t_b;\beta,t)+S(\beta,t;\alpha,t_a)=S(\gamma,t_b;\alpha,t_a)\ . \tag{A58}$$

Indeed, for β a critical point the piecewise classical path characterized by (α,t_a), (β,t), and (γ,t_b) must be the classical path characterized by $(\alpha,t_a)(\gamma,t_b)$. The additive property of the different action functions follows from (A17).

It remains to prove that, for β a critical point,

$$\det\partial^2S(\gamma,t_b;\alpha,t_a)/\partial\gamma\,\partial\alpha = -\det\partial^2S(\gamma,t_b;\beta,t)/\partial\gamma\,\partial\beta\{\det[\partial^2S(\gamma,t_b;\beta,t)/\partial\beta\,\partial\beta+\partial^2S(\beta,t;\alpha,t_a)/\partial\beta\,\partial\beta]\}^{-1}\times\det\partial^2S(\beta,t;\alpha,t_a)/\partial\beta\,\partial\alpha\ . \tag{A59}$$

If the critical point is not degenerate, the most direct proof[25] of (A59) consists in computing the second derivatives of both sides of (A58) when β is a function of α and γ. This can be done in different ways, by changing the order of differentiation and using, or not using, the fact that the derivatives of (A58) with respect to the components of β vanishes. The resulting equation (A59) is meaningless if β is a degenerate critical point. We shall instead give Jacobi field identities which are equivalent to (A59), but which remain valid when β is a degenerate critical point. The correspondence between the Jacobi field identities and (A59) follows from (A26), (A27), (A30), (A31), (A34), (A35), (A37), and (A38), where we have obtained the Hessian of the action functions in terms of the Jacobi fields.

(a) If $\alpha=q(t_a)$, $\beta=q(t)$, and $\gamma=q(t_b)$, then (A59) can be written

$$M(t_b,t_a)=M(t_b,t)[\tilde{K}(t,t_a)M(t_a,t)-\tilde{K}(t,t_b)M(t_b,t)]^{-1}M(t,t_a) . \tag{A60}$$

This equation follows from

$$\tilde{K}(t,t_a)M(t_a,t)-\tilde{K}(t,t_b)M(t_b,t)=M(t,t_a)J(t_a,t_b)M(t_b,t) , \tag{A61}$$

when the left-hand side is invertible. Equation (A61) is valid whether or not the left-hand side is invertible.

Proof of (A61). From

$$-J(t,s)=J(t,t_a)M(t_a,t_b)J(t_b,s)+J(t,t_b)M(t_b,t_a)J(t_a,s) , \tag{A62}$$

and if $t=s$,

$$J(t,t_a)M(t_a,t_b)J(t_b,t)=-J(t,t_b)M(t_b,t_a)J(t_a,t) . \tag{A63}$$

Taking the derivative of (A62) with respect to t, and setting $t=s$, one obtains

$$-\mathbb{1}=\tilde{K}(t,t_a)M(t_a,t_b)J(t_b,t)+\tilde{K}(t,t_b)M(t_b,t_a)J(t_a,t) ,$$

which, inserted in (A63), gives

$$\tilde{K}(t,t_a)-\tilde{K}(t,t_b)M(t_b,t)J(t,t_a)=-M(t,t_b)J(t_b,t_a) .$$

Then

$$\tilde{K}(t,t_a)M(t_a,t)-\tilde{K}(t,t_b)M(t_b,t)=-M(t,t_b)J(t_b,t_a)M(t_a,t) . \tag{A64}$$

(b) If $\alpha=p(t_a)$, $\beta=q(t)$, and $\gamma=p(t_b)$, then (A59) can be written

$$P(t_b,t_a)=N(t_b,t)[-L(t,t_a)N(t_a,t)-L(t,t_b)N(t_b,t)]^{-1}\tilde{N}(t,t_a) . \tag{A65}$$

This equation follows from

$$L(t,t_a)N(t_a,t)-L(t,t_b)N(t_b,t)=\tilde{N}(t,t_b)L(t_b,t_a)N(t_a,t) \tag{A66}$$

when the left-hand side is invertible. Equation (A65) is valid whether or not the left-hand side is invertible.

Proof of (A66). Taking the derivative of (A44) with respect to t, and setting $t=s$ gives

$$L(t,t_a)P(t_a,t_b)\tilde{K}(t_b,t)-L(t,t_b)\tilde{P}(t_b,t_a)\tilde{K}(t_a,t)=\mathbb{1} . \tag{A67}$$

Setting $t=s$ in (A44) gives

$$\tilde{P}(t_b,t_a)\tilde{K}(t_a,t)=N(t_b,t)K(t,t_a)P(t_a,t_b)\tilde{K}(t_b,t) , \tag{A68}$$

which, inserted in (A67), gives

$$[L(t,t_a)-L(t,t_b)N(t_b,t)K(t,t_a)]P(t_a,t_b)\tilde{K}(t_b,t)=\mathbb{1} ,$$

from which (A66) follows.

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[1]This paper uses methods developed by C. DeWitt-Morette, A. Maheshwari, and B. Nelson, Phys. Rep. 50, 255 (1979). The notation is similar except for the Legendre metric tensor, which used to be $g_{\alpha\beta}=m^{-1}\partial^2L/\partial\dot{q}^\alpha\partial\dot{q}^\beta$, and is now chosen to be $g_{\alpha\beta}(q(t))=\partial^2L/\partial\dot{q}^\alpha(t)\partial\dot{q}^\beta(t)$. Thus $p_\alpha=g_{\alpha\beta}\dot{q}^\beta$.

[2]The results are valid for arbitrary Lagrangians or arbitrary Riemannian manifolds. See Ref. 1 for the appropriate changes, e.g., Eq. (4) is to be replaced by Ref. 1, Eq. (3.7), etc. For systems with time-dependent metric and velocity-dependent potentials, use the results of B. Nelson and B. Sheeks, J. Math. Phys. 22, 1944 (1981); Commun. Math. Phys. 84, 515 (1982).

[3]If, as it will turn out, $I\sim\hbar^n$, $\lim_{\hbar=0}$ is to be understood as the dominating term when $\hbar$ tends to 0.

[4]See the Appendix, pp. 14—15. This choice of initial wave function and the analysis of the corresponding classical flow has been used in K. D. Elworthy and A. Truman, J. Math. Phys. 22, 2144 (1981).

[5]The case when the classical flows are caustic forming is discussed in C. DeWitt-Morette, B. Nelson, and T.-R. Zhang, second following paper, Phys. Rev. D 28, 2526 (1983).

[6]See Ref. 1 for the detailed calculations leading from (4) and (5) to (10) and (11).

[7]W. Gordon, Z. Schweisstech. 48, 180 (1928). Illustrated by A. Young and translated. Center for Relativity, University of Texas, Austin.

[8]See the Appendix, Eqs. (A28a) and (A32a). This property would not be true without the end-point contributions.

[9]$q:[t_a,t_b]\to R^n$ by $q_a:[t_a,t]\to R^n$, $q_b:[t,t_b]\to R^n$.

[10]See, for instance, J. Milnor, *Morse Theory*, Annals of Math. Studies No. 51 (Princeton University Press, Princeton, New Jersey, 1969), pp. 5—6.

[11]See J. Milnor, *Morse Theory*, Ref. 10, p. 7.

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

[13]L. R. I. Schiff, *Quantum Mechanics*, 3rd ed. (McGraw-Hill, New York, 1968).

[14]Jacobi fields and related topics is Appendix B in Ref. 1. To-

gether with Ref. 1, note III added in proof, Ref. 1, pp. 323—328, and C. DeWitt-Morette, Ann. Phys. (N.Y.) 97, 367 (1976); 101, 682 (E) (1976), it provides an extensive discussion of Jacobi fields in the context of path integration. In the present appendix, we give without proof some formulas derived in these references, and derive new results necessary for the analysis of conservation laws.

[15]Unless otherwise stated, we use the norm induced by g, hence $p_\mu = g_{\mu\nu}\dot{q}^\nu$.

[16]M. Mizrahi, Ph.D. thesis, University of Texas at Austin, 1975 (unpublished); report, Center for Naval Analysis of the University of Rochester, Arlington, VA.

[17]For computing path integrals (A45) and (A46) with initial or final wave functions of type (A49), it is convenient to choose K such that

$$dK_{\mu\nu}(t,t_a)/dt\,|_{t=t_a} = \partial^2 S_a(q(t_a))/\partial a^\mu(t_a)\partial q^\nu(t_a) .$$

See Ref 1, p. 266.

[18]M. Mizrahi, J. Math. Phys. 20, 844 (1979); B. J. Sheeks, Ph.D. thesis, The University of Texas, 1980 (unpublished).

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

[20]See Ref. 1, p. 323—327.

[21]The time derivative of G need not vanish on the boundary. See (A6) for systems when the time derivative of K does not vanish on the boundary: velocity-dependent potentials, time-dependent metric, initial or final wave functions of type (A49) other than plane waves.

[22]See Ref. 1, pp. 291 and 366. There are four different Feynman-Kac formulas solving (in the case of Wiener integrals) the diffusion equation, the forward and backward Fokker-Planck equations, and what might be called a backward-diffusion equation. There are generalizations of these Feynman-Kac formulas corresponding to other types of transitions; see, in particular, R. L. Hudson, P. D. F. Ion, and K. R. Parthasarathy, Commun. Math. Phys. 83, 261 (1982); and if one considers the discrete versions there are many more.

[23]For time-dependent metrics and velocity-dependent potentials, one can use Nelson and Sheek's results (see Ref. 2).

[24]R. P. Feynman and A. R. Hibbs, *Quantum Mechanics and Path Integrals* (McGraw-Hill, New York, 1965).

[25]B. S. DeWitt, private communication.