Structural connections between two semiclassical approximations: The WKB and Wigner-Kirkwood approximations

T. A. Osborn and F. H. Molzahn
Department of Physics, University of Manitoba, Winnipeg, Manitoba, Canada R3T2N2
(Received 9 October 1985)

The mutual consistency and structural interconnection between the Wentzel-Kramers-Brillouin (WKB) and Wigner-Kirkwood (WK) semiclassical approximations is investigated for nonrelativistic N-particle systems, with mutual scalar interactions and coupling to an external time-varying electromagnetic field. The generalized WK expansion of the propagator $\langle x \mid U(t,s) \mid y \rangle$ is obtained from a large-mass expansion of the higher-order WKB approximation. Two techniques are described for computing the WK coefficient functions. One relies on a large-mass expansion of classical paths and the transport representation of the WKB approximation; the other is recursive in nature. For time-independent Hamiltonians H the standard WK expansion of the heat kernel $\langle x \mid e^{-\beta H} \mid y \rangle$ is recovered.

I. INTRODUCTION

Semiclassical behavior of a quantum system can result from either of two asymptotic limits. One may assume that Planck's constant h is small and study the limit $h \to 0$; or the particle mass m may be taken as large and the associated limit $m \to \infty$ investigated. Each of these semiclassical mechanisms has a large and active literature. The characterization of quantum dynamics as $h \to 0$ leads to the Wentzel-Kramers-Brillouin (WKB) approximation in the form found initially in the work of Birkhoff.[1] The $m \to \infty$ asymptotic expansion can be shown[2] to be the limiting mechanism responsible for the Wigner-Kirkwood approximation.[3,4] In this paper we investigate the mutual consistency and the structural interconnections between these two nonperturbative semiclassical approximations.

The physical systems we consider are defined by the class of time-dependent Hamiltonians of the form

$$H(x,p,t) = \frac{1}{2m}[p - A(x,t)]^2 + v(x,t) . \quad (1.1)$$

Here x is the generic coordinate vector in $\mathbb{R}^n$ that determines the position of all of the system particles, p is the momentum conjugate to x, and t is the time variable. The interaction structure, responsible for nontrivial dynamics, is given by a time-dependent vector field A and scalar field v. Time evolution of a state vector ψ, in Hilbert space $\mathscr{H} = L^2(\mathbb{R}^n)$, is determined by the time-dependent Schrödinger equation,

$$i\hbar \frac{\partial}{\partial t}\psi(x,t) = H(x, -i\hbar\nabla_x, t)\psi(x,t) . \quad (1.2)$$

The Schrödinger problem (1.2) may be identified with the N-body quantum problem if each point particle is spinless, moves in three dimensions (so that $n = 3N$), and has mass m. The presence of the vector potential in (1.1) means that the Hamiltonian $H(x,p,t)$ describes the nonrelativistic dynamics of a finite collection of particles that mutually interact through scalar fields and couple via the Lorentz force to a temporally and spatially varying external electromagnetic field.

In order to clarify the statement of our problem and to illustrate the basic ideas in the simplest possible context let us restrict our discussion (in the remainder of this Introduction) to the static scalar field case, i.e., $A(x,t) = 0$ and $v(x,t) = v(x)$. In this circumstance Schrödinger's equation becomes

$$\left[-\frac{\hbar^2}{2m}\Delta_x - i\hbar\frac{\partial}{\partial t} + v(x) \right]\psi(x,t) = 0 . \quad (1.3)$$

Time evolution of the system is then determined by the one-parameter group $\{e^{-itH/\hbar} : t \in \mathbb{R}\}$ of unitary operators acting in $\mathscr{H}$. The related quantum propagator is defined as the integral kernel (coordinate-space Dirac matrix element), $\langle x \mid e^{-itH/\hbar} \mid y \rangle$, of the evolution operator. With this terminology the Cauchy initial data problem for Eq. (1.3) assumes the following standard form. Suppose state vector ψ is equal to the initial data function ϕ in $\mathscr{H}$ at time s; then the solution of (1.3) is expressed in terms of the propagator by the integral

$$\psi(x,t) = \int \langle x \mid e^{-i(t-s)H/\hbar} \mid y \rangle \phi(y) d^n y . \quad (1.4)$$

Both the generalized WKB method and the Wigner-Kirkwood (hereafter WK) approach may be used to obtain nonperturbative (infinite order in the potential) approximations for the propagator. Let us compare the basic forms assumed by these two approximations for the static scalar field problem. Consider first the WKB approximation. Here the propagator is represented asymptotically as $h \to 0$ by

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$$\langle x \,|\, e^{-i(t-s)H/\hbar} \,|\, y \rangle \sim \left[\frac{m}{2\pi i \hbar (t-s)} \right]^{n/2} e^{(i/\hbar)S(x,t;y,s)} \exp[\Psi(x,t;y,s)] \,. \tag{1.5}$$

The function S is the classical action [for system $H(x,p,t)$] that appears in the statement of Hamilton's least-action principle. Suppose $q(\tau)$ is the unique solution to the Euler-Lagrange equations for the two-point boundary-value problem in which the classical system starts with configuration y at time s and arrives at configuration x at time $t>s$, then

$$S(x,t;y,s) = \int_s^t \left[\frac{m}{2}\dot{q}(\tau)^2 - v(q(\tau)) \right] d\tau \,. \tag{1.6}$$

Here, the (Newtonian) dot indicates ordinary differentiation. Clearly S determines the rapidly oscillating phase behavior (as $h \to 0$) of the propagator, whereas the complex-valued Ψ contains the nontrivial amplitude dependence. The function Ψ is smooth in $\hbar$ and allows a small $\hbar$ expansion

$$\Psi = \psi_1 + (i\hbar)\psi_2 + (i\hbar)^2\psi_3 + \cdots \,. \tag{1.7}$$

A simple procedure called the transport method allows the determination of the values of ψ_j in terms of the action function S.

The large-mass (or WK) approximation of the time-evolution kernel is given by the $m \to \infty$ asymptotic representation

$$\langle x \,|\, e^{-i(t-s)H/\hbar} \,|\, y \rangle \sim \left[\frac{m}{2\pi i \hbar (t-s)} \right]^{n/2} \exp\left[\frac{im(x-y)^2}{2\hbar(t-s)} + \frac{t-s}{i\hbar} \int_0^1 v(\hat{\xi})d\xi \right] \left[1 + \frac{1}{m}T_1 + \frac{1}{m^2}T_2 + \cdots \right] , \tag{1.8}$$

where the argument of the coefficient functions T_j is $(x,t;y,s)$. The v-dependent term in the exponential is the mean value of the potential v integrated over a linear path in $\mathbb{R}^n$ having end points x and y, i.e.,

$$\hat{\xi} \equiv y + \xi(x-y), \quad \xi \in [0,1] \,. \tag{1.9}$$

It is evident that expansions (1.5) and (1.8) represent the asymptotic approximations associated with two similar problems in singular perturbation theory.[5] In singular perturbation theory one examines the behavior of the solutions of a partial differential equation as a function of a vanishing parameter appearing in front of the highest-order differential term. In the $m \to \infty$ case we see that the multiplier of the Laplacian term in (1.3) vanishes. In the $h \to 0$ problem the singularity is somewhat more severe in that both the Laplacian and time-derivative multipliers vanish. It is a common occurrence in singular perturbation theory that the behavior of the solution in the small parameter is highly singular. Both (1.5) and (1.8) exhibit essential singularities in their respective small parameters, i.e., h and m^{-1}. Only after the precise mathematical structure of the essential singularity has been determined is it then possible to carry out a small-parameter asymptotic expansion in the neighborhood of the singular point.

Expansions (1.5) and (1.8) are nonperturbative in character because in both the leading term is infinite order in the potential v, and thus both are capable of accurate predictions in the case of very strong interactions. For the large-mass expansion problem a combinatorial method[6] based on connected simple graphs gives a procedure for obtaining in closed analytical form all of the coefficient functions T_j. In the WKB method the higher-order coefficient terms ψ_j are determined from a special type of one-dimensional recurrence relation[1,7] in terms of the action S. The WKB approximation has been the subject of extensive study[8–41] primarily because the functions appearing in the expansion are all determined from classical mechanics. Thus (1.5) allows a detailed comparison of quantum and classical dynamics. On the other hand, the WK approximation is appealing because the coefficients T_j are so simple and are correspondingly easy to evaluate.[6,41–59] In particular, it has been widely used in quantum statistical mechanics.[60–65] Note if $t \to \hbar\beta/i$ then (1.3) becomes the Bloch equation describing the system with Hamiltonian $H(x,p)$ that has inverse temperature $\beta > 0$. In this circumstance expansion (1.8) describes the coordinate-space Dirac matrix elements of the canonical density operator $e^{-\beta H}$.

Since the parameter m does not occur in the transformation $t \to \hbar\beta/i$, the analytic structures of $\langle x \,|\, e^{-itH/\hbar} \,|\, y \rangle$ and $\langle x \,|\, e^{-\beta H} \,|\, y \rangle$ in m^{-1} should be equivalent. Further, the heat kernel (in the $A=0$ case) only depends[6] on $\hbar$ and m through the quantity $\hbar^2/2m$. Hence, a large-mass expansion of the heat kernel determines at once its form as $\hbar \to 0$ (i.e., the traditional[3,4] Wigner-Kirkwood expansion).

The basic idea in this paper is that one may obtain the WK approximation for the propagator from an appropriate infinite-mass expansion of the WKB approximation. From Eqs. (1.5)—(1.7), it is apparent we must determine the $m \to \infty$ expansion of the action S and the expansion of the associated coefficient functions ψ_j. The mass dependence of S has two sources. First, there is the explicit mass variable in the formula for the Lagrangian; second, there is an implicit mass dependence in the classical path $q(\tau)$. We characterize the mass dependence of $q(\tau)$ by a Taylor series in m^{-1}

$$q(\tau) = \rho_0(\tau) + \sum_{j=1}^{\infty} m^{-j}\rho_j(\tau) \,. \tag{1.10}$$

Since $q(\tau)$ describes the solution of the two-fixed-end-point problem in classical mechanics, the leading term $\rho_0(\tau)$ represents a linear trajectory from y to x having constant velocity $(x-y)/(t-s)$. Once the higher coefficients $\rho_j(\tau)$ have been found the large-mass behavior of S will be well defined. Proceeding in this fashion, and upon employing the transport method, it becomes possible to determine closed-form off-diagonal $(x \neq y)$ expressions for the WK coefficients T_j. This method of obtaining the WK expansion from the WKB expansion via a large-mass expansion has wide applicability since it requires only that the dynamical quantum problem arise from a well-defined Lagrangian with an analytic dependence on the mass parameter.

When specialized to the density $\langle x | e^{-\beta H} | x \rangle$, the present method bears some conceptual similarity with the work of Miller.[57] He obtained a WK expansion of the density by combining the lowest-order WKB approximation with the short-time expansion of a classical trajectory. With that approach a number of the lower-order WK coefficients are correctly determined, but the higher-order coefficients are incorrect because of the incomplete WKB approximation used.

Semiclassical asymptotic approximations have, in general, three basic features. These are (i) the analytic structure (particularly the singular behavior) in the small parameter, (ii) the construction of formulas for the higher correction terms, and (iii) the convergence properties of the approximating series (e.g., the determination of the order and uniformity of the asymptotic series together with estimates that bound the total error). This last aspect is by far the most intractable feature of these approximations to understand, and only a limited number of results are available. However, the scalar field problem of (1.3) is well understood in all three of the above aspects. Fujiwara[36] gives coefficient expressions and error term bounds for the WKB propagator approximation, and Osborn[2] finds error term bounds for the WK approximation that are valid for both the time evolution and temperature (Bloch equation) realizations of the problem.

The analysis in this paper will establish the linkage between WKB and WK approximations in a formal fashion and so will not give estimates of the total error. All of our mathematical derivations are of a heuristic nature, and throughout it is assumed that series expansions have meaning and are at least asymptotically convergent.

Section II describes the large-mass expansion of the classical path $q(\tau)$. In Sec. III the WKB approximation is reviewed and the transport method is used to obtain the behavior of the higher-order corrections to the first-order WKB formula. By combining the results of the large-mass path expansion and the transport recurrence relations, Sec. IV shows how the WK expansion can be obtained from the $m \to \infty$ behavior of the WKB approximation. The Appendix discusses an alternate large-mass expansion method which does not employ any direct reference to classical paths.

II. THE LARGE-MASS EXPANSION OF THE CLASSICAL PATH

The purpose of this section is to analyze the inverse-mass expansion (1.10) of the classical path. After defining the general Hamiltonian system to be considered, we motivate the form of the expansion and show how to solve for all the coefficients $\rho_k(\tau)$ recursively. The first few of these coefficients are calculated explicitly, since they will be needed in Sec. IV to illustrate the bridge between the WK and WKB methods.

We investigate classical paths of a system described by a Lagrangian L of the form

$$L(x,\dot{x},t)=\frac{m}{2}\dot{x}^2+A(x,t)\cdot\dot{x}-v(x,t)\,, \tag{2.1}$$

where it is assumed throughout that the fields A,v and their derivatives are smooth bounded functions. Physically (2.1) describes a nonrelativistic classical system of N point masses m_i having charges $Q_i (i=1 \sim N)$ that move in three dimensions, if $n=3N$. For an arbitrary mass parameter m, define the mass ratios $\mu_i=m_i/m$, and let $r^i/\mu_i^{1/2}$ be the position of the ith particle in $\mathbf{R}^3$; then

$$x=(r^1,\ldots,r^N)\equiv \bigtimes_{i=1}^{N} r^i\,,$$

where $\bigtimes$ denotes a Cartesian product. Suppose the particles' mutual interaction is described by a smooth total potential energy $\hat{v}(x,t)$, and that they couple to external electric and magnetic fields described by a magnetic vector potential $\mathscr{A}$ and scalar potential ϕ so

$$E=-\nabla\phi-\partial\mathscr{A},\quad B=\nabla\times\mathscr{A}\,.$$

Then (2.1) describes this system provided we take

$$A(x,t)=\bigtimes_{i=1}^{N} Q_i\mu_i^{-1/2}\mathscr{A}(\mu_i^{-1/2}r^i,t)$$

and

$$v(x,t)=\sum_{i=1}^{N} Q_i\phi(\mu_i^{-1/2}r^i,t)+\hat{v}(x,t)\,.$$

The large mass limit of our system is to be understood as follows. We consider the ratios μ_i [and hence A,v in (2.1)] to be fixed, while the explicit m in (2.1) is allowed to become large. This amounts to considering a family (with continuous index m) of dynamics problems with fixed mass ratios among the particles (μ_i/μ_j), and which reduce to the original dynamics problem when m assumes the value used to define the fixed $\{\mu_i\}$. This interpretation differs from other useful large mass limits to be found in the literature, for example the Born-Oppenheimer[66] approximation in which the masses of only some of the system particles are allowed to become large. In the present scheme, all particle masses become large in unison, as is seen from the relations $m_i=\mu_i m$ (μ_i fixed, $m\to+\infty$).

Let p be the momentum conjugate to x. Then the Hamiltonian (1.1) is that associated with Lagrangian (2.1), and system dynamics is described by Hamilton's equations

$$\dot{q}(\tau)=\nabla_2 H(q(\tau),p(\tau),\tau)\,, \tag{2.2a}$$

$$\dot{p}(\tau)=-\nabla_1 H(q(\tau),p(\tau),\tau)\,. \tag{2.2b}$$

Combining these gives Newton's equation for the classical path $q(\tau)$

$$\ddot{q}_\alpha(\tau)=\frac{1}{m}[f_\alpha(q(\tau),\tau)+\dot{q}_\beta(\tau)F_{\alpha\beta}(q(\tau),\tau)] , \quad (2.3)$$

where we have introduced

$$f_\alpha=-\nabla^\alpha v-\partial A_\alpha , \quad (2.4a)$$

$$F_{\alpha\beta}=\nabla^\alpha A_\beta-\nabla^\beta A_\alpha . \quad (2.4b)$$

Our notation is as follows. First, greek indices $\alpha,\beta,\ldots$ range from 1 to n, and we employ the summation convention on repeated greek indices in a term [e.g., (2.3)]. Concerning derivatives, ∇ denotes differentiation with respect to a vector argument, and ∂ with respect to a scalar argument. If there is more than one argument of either type, we use ∇_j (or ∂_j) to denote differentiation with respect to the jth vector (or scalar) argument (cf. Hamilton's equations). Finally ∇_j^β denotes the βth component of this gradient. (The location of indices carries no covariance implications.)

Equation (2.3) has the form of a Lorentz force law for the N-body system. If $N=1$ and $\hat{v}=0$ it is easily checked that it reduces to $m\ddot{q}=Q(E+\dot{q}\times B)$. The quantities $f_\alpha, F_{\alpha\beta}$ are all gauge invariant (this topic will be discussed in Sec. III).

The classical action $S(x,t;y,s)$ which occurs in the WKB approximation requires the solution to (2.3) subject to the two-point boundary condition

$$q(s)=y,\ \ q(t)=x\ \ (s<t) , \quad (2.5)$$

where x,y are fixed configurations. Assume a unique solution $q(\tau)=q(\tau;x,t;y,s)$, $s\le\tau\le t$, to this problem exists. This is generally the case for smooth bounded potentials if $t-s$ is small enough.[36] Write

$$q=\rho_0+\eta , \quad (2.6)$$

where

$$\rho_0(\tau)=y+\frac{\tau-s}{t-s}(x-y)=\hat{\xi} , \quad (2.7)$$

where $\xi=(\tau-s)/(t-s)$. Note that ρ_0 is the linear path in $\mathbf{R}^n$ satisfying (2.5), and that ρ_0 solves (2.3) if the right-hand side vanishes (free motion or infinite mass limits). Formulas (2.6) and (2.7) are essentially a definition of η. Since the boundary conditions on q are already satisfied by ρ_0, we require

$$\eta(s)=\eta(t)=0 . \quad (2.8)$$

Suppose now that the functions $\{f_\alpha,F_{\alpha\beta}\}$ are bounded on the domain $\mathbf{R}^n\times[s,t]$. Consider the formal limit $m\to\infty$ in (2.3). As m increases, the path q which depends on m changes. Assuming that $\dot{q}$ remains bounded with respect to this dependence in a neighborhood of $m^{-1}=0$, one finds $\ddot{q}(\tau)\to 0$ as $m\to\infty$. Integrating this twice and applying (2.5) shows $q(\tau)\to\rho_0(\tau)$ and hence $\eta(\tau)\to 0$, as $m\to\infty$. Motivated by these considerations we seek an expansion of η of the form

$$\eta(\tau)=\sum_{j=1}^{\infty} m^{-j}\rho_j(\tau) , \quad (2.9)$$

where the coefficients $\rho_j(\tau)$ are mass independent. If (2.8) is to hold for all m, we require

$$\rho_j(s)=\rho_j(t)=0\ \ (j\ge 1) . \quad (2.10)$$

We have thus arrived at the form (1.10) of the m^{-1} expansion of the classical path q about the linear path ρ_0 representing "free" motion of a system subject to constraint (2.5).

The next objective is to solve for the coefficients ρ_j using a simple recursive method. The basic idea is to substitute (1.10) into (2.3); then comparing powers of m^{-1} yields equations of motion for ρ_j which may be solved using a simple one-dimensional Green's function. Let us substitute (2.6) into (2.3), and express the resulting force terms as Taylor series. We obtain

$$f_\alpha(q,\tau)=f_\alpha(\rho_0+\eta,\tau)=e^{\eta\cdot\nabla}f_\alpha(\rho_0,\tau)$$

and similarly

$$F_{\alpha\beta}(q,\tau)=e^{\eta\cdot\nabla}F_{\alpha\beta}(\rho_0,\tau) .$$

Here ∇ acts on the vector argument of f_α, or $F_{\alpha\beta}$, as usual, and we have suppressed the τ argument of the path functions for brevity. Insert (1.10) and the above into (2.3) to obtain

$$\sum_{j=1}^{\infty} m^{-j}\ddot{\rho}_{j\alpha}=\frac{1}{m}e^{\eta\cdot\nabla}f_\alpha(\rho_0,\tau)+\frac{1}{m}\left[\sum_{j=0}^{\infty} m^{-j}\dot{\rho}_{j\beta}\right]e^{\eta\cdot\nabla}F_{\alpha\beta}(\rho_0,\tau) , \quad (2.11)$$

where we used $\ddot{\rho}_0=0$, and $\rho_{j\alpha}$ is the αth component of ρ_j.

In order to equate common powers of m^{-1} in (2.11), employ (2.9) to write

$$e^{\eta\cdot\nabla}=\prod_{j=1}^{\infty}\exp(m^{-j}\rho_j\cdot\nabla)=\sum_{n_1=0}^{\infty}\cdots\sum_{n_\infty=0}^{\infty}\prod_{j=1}^{\infty}(n_j!)^{-1}(\rho_j\cdot\nabla)^{n_j}m^{-jn_j} .$$

Hence the coefficient of m^{-p} in $e^{\eta\cdot\nabla}$ is

$$\sum_{(n_j)}^{p}\left[\prod_{j=1}^{p}(n_j!)^{-1}(\rho_j\cdot\nabla)^{n_j}\right] , \quad (2.12)$$

where the sum specified by $\sum_{(n_j)}^p$ is defined as follows: If $p=0$, then $\sum_{(n_j)}^p[\ldots]\equiv 1$; if $p\geqq 1$, then sum over all the p-tuples of non-negative integers $(n_j)\equiv(n_1,\ldots,n_p)$ which satisfy the constraint

$$\sum_{j=1}^{p} jn_j=p .$$

With (2.12) we can equate the coefficient of $m^{-(p+1)}$, where $p\geqq 0$, in (2.11) to obtain

$$\ddot{\rho}_{p+1,\alpha}=\sum_{(n_j)}^{p}\left[\prod_{j=1}^{p}(n_j!)^{-1}(\rho_j\cdot\nabla)^{n_j}\right]f_\alpha(\rho_0,\tau)$$
$$+\sum_{r=0}^{p}\dot{\rho}_{p-r,\beta}\left[\sum_{(n_j)}{}'\prod_{j=1}^{r}(n_j!)^{-1}(\rho_j\cdot\nabla)^{n_j}\right]F_{\alpha\beta}(\rho_0,\tau). \tag{2.13}$$

Notice the right-hand side of (2.13) involves only $\rho_0,\ldots,\rho_p$. Since ρ_0 is known, we may solve recursively for any ρ_{p+1}. Specifically, the problem for $\rho_{p+1,\alpha}$ is of the form

$$\frac{d^2}{d\tau^2}\rho_{p+1,\alpha}(\tau)=h(\tau)$$

along with the homogeneous boundary conditions (2.10). The Green's function solution for this problem has the standard form

$$\rho_{p+1,\alpha}(\tau)=-\int_s^t d\tau'(\tau_<-s)(t-\tau_>)(\Delta t)^{-1}h(\tau')$$

where $\tau_<\equiv\min\{\tau,\tau'\}$, $\tau_>\equiv\max\{\tau,\tau'\}$, and $\Delta t=t-s$. A change of variable to the unit interval allows us to scale out the trivial dependences on Δt. Upon setting $\tau=s+\xi\Delta t$, $0\le\xi\le1$, we find

$$\rho_{p+1,\alpha}(s+\xi\Delta t)=-(\Delta t)^2\int_0^1 d\xi' g(\xi,\xi')h(s+\xi'\Delta t) \tag{2.14}$$

where g is the unit-interval Green's function

$$g(\xi,\xi')\equiv\xi_<(1-\xi_>)\ . \tag{2.15}$$

As an illustration of the use of (2.13) and (2.14) let us compute ρ_1 and ρ_2 (both of these are required in Sec. III). Start with ρ_1. In this case (2.13) with $p=0$ becomes

$$\ddot{\rho}_{1\alpha}=f_\alpha(\rho_0,\tau)+\dot{\rho}_{0\beta}F_{\alpha\beta}(\rho_0,\tau)\ .$$

Notice that $\dot{\rho}_0=(x-y)/\Delta t$ (constant velocity), and that $\rho_0(s+\xi'\Delta t)$ is $\hat{\xi}'$. Then (2.14) yields

$$\rho_{1\alpha}(s+\xi\Delta t)=-(\Delta t)^2\int_0^1 d\xi' g(\xi,\xi')\left[f_\alpha(\hat{\xi}',s+\xi'\Delta t)+\frac{(x-y)_\beta}{\Delta t}F_{\alpha\beta}(\hat{\xi}',s+\xi'\Delta t)\right].$$

Observe that both the space and time arguments of $f_\alpha,F_{\alpha\beta}$ are integrated along a linear path from the initial (y,s) to the final (x,t) value. This will occur repeatedly in our analysis, so it is convenient to introduce the space-time linear path for $0\le\xi\le1$:

$$\tilde{\xi}\equiv(y+\xi(x-y),s+\xi(t-s))=(\hat{\xi},s+\xi\Delta t)\ . \tag{2.16}$$

Also, the quantity in large parentheses above will occur often so we denote it by

$$\omega_\alpha(z,\tau)\equiv\omega_\alpha(z,\tau;(x-y)/\Delta t)$$
$$=f_\alpha(z,\tau)+\frac{(x-y)_\beta}{\Delta t}F_{\alpha\beta}(z,\tau)\ . \tag{2.17}$$

where $(z,\tau)\in\mathbb{R}^{n+1}$. For future reference we note the composition law ($\lambda\in[0,1]$),

$$\omega_\alpha(\tilde{\lambda})\,|_{(x,t)=\tilde{\xi}}=f_\alpha(\tilde{\gamma})+\frac{\xi(x-y)_\beta}{\xi\Delta t}F_{\alpha\beta}(\tilde{\gamma})=\omega_\alpha(\tilde{\gamma})\ , \tag{2.18}$$

where $\gamma=\lambda\xi$. The values $\omega_\alpha(\tilde{\xi})$ represent the Lorentz force acting on a system moving on the linear trajectory $\rho_0(\tau)$. With these notations the result for ρ_1 may be restated as

$$\rho_{1\alpha}(s+\xi\Delta t)=-(\Delta t)^2\int_0^1 d\xi' g(\xi,\xi')\omega_\alpha(\tilde{\xi}')\ . \tag{2.19}$$

Now consider the form taken by ρ_2. Equation (2.13) with $p=1$ reads

$$\ddot{\rho}_{2\alpha}=\rho_1\cdot\nabla\omega_\alpha(\rho_0,\tau)+\dot{\rho}_{1\beta}F_{\alpha\beta}(\rho_0,\tau)\ . \tag{2.20}$$

Here, as usual, ∇ acts on the vector argument of ω_α. This would correspond to ∇_z in (2.17), so ∇ acts on $f_\alpha,F_{\alpha\beta}$ (and not x). The velocity term $\dot{\rho}_{1\beta}$ follows from (2.19) upon using $d/d\tau=(1/\Delta t)(d/d\xi)$,

$$\dot{\rho}_{1\beta}(s+\xi\Delta t)=-\Delta t\int_0^1 d\xi'\partial_1 g(\xi,\xi')\omega_\beta(\tilde{\xi}')\ . \tag{2.21}$$

Integrating (2.20), as in (2.14), and substituting (2.19), (2.21) yields

$$\rho_{2\alpha}(s+\xi\Delta t)=(\Delta t)^4\int_0^1 d\xi_1\int_0^1 d\xi_2\, g(\xi,\xi_1)\omega_\beta(\tilde{\xi}_2)[g(\xi_1,\xi_2)\nabla^\beta\omega_\alpha(\tilde{\xi}_1)+\partial_1 g(\xi_1,\xi_2)(\Delta t)^{-1}F_{\alpha\beta}(\tilde{\xi}_1)]\ . \tag{2.22}$$

It should now be evident how one proceeds to solve for the general coefficient ρ_j in (1.10).

III. TRANSPORT EQUATIONS

It is the transport method that makes the determination of the higher-order correction terms to the WKB approximation possible. In a notation suitable for the further development of the large mass expansion we give an account of the transport recurrence relations and their solutions which provide expressions for ψ_j. The use of the transport method in quantum mechanics apparently originates in the work of Birkhoff,[1] although it was rediscovered by Luneburg[7] in an optics context. This section concludes with a discussion of the gauge transformation properties of the WKB representation of the propagator.

From a partial differential equation perspective the quantum propagator is the solution of the time-dependent Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\langle x\mid U(t,s)\mid y\rangle = H(x,-i\hbar\nabla_x,t)\langle x\mid U(t,s)\mid y\rangle \tag{3.1}$$

subject to the δ-function initial condition imposed at an arbitrary starting time s,

$$\langle x\mid U(t,s)\mid y\rangle \to \delta(x-y) \quad \text{as } t\to s\ . \tag{3.2}$$

The notation adopted here for the propagator reflects the fact that if the Hamiltonian is time dependent then the evolution operator, $U(t,s)$, depends independently on t and s and is not a one-parameter group in the time displacement variable $t-s\equiv\Delta t$. The quantum Hamiltonian corresponding to (1.1) and Lagrangian (2.1) is

$$\begin{aligned}H(x,-i\hbar\nabla_x,t)=&\frac{-\hbar^2}{2m}\Delta_x+\frac{i\hbar}{m}A(x,t)\cdot\nabla_x\\&+\frac{i\hbar}{2m}\nabla\cdot A(x,t)+\frac{1}{2m}\mid A(x,t)\mid^2\\&+v(x,t)\ .\end{aligned} \tag{3.3}$$

The WKB approximation for $\langle x\mid U(t,s)\mid y\rangle$ may be constructed as follows. The first step is to make an ansatz about the essential singularity structure in the variable $\hbar$ of the propagator, namely

$$\langle x\mid U(t,s)\mid y\rangle = \left[\frac{m}{2\pi i\hbar\Delta t}\right]^{n/2}\exp\left[\frac{i}{\hbar}\mathscr{S}+\Psi\right], \tag{3.4}$$

where the phase function $\mathscr{S}$ is assumed real valued, dependent upon $x,t;y,s$ and independent of $\hbar$. The less singular complex-valued amplitude and phase correction Ψ is assumed to be smooth in $\hbar$ and to admit a small-$\hbar$ Taylor-series expansion (1.7).

Insertion of (3.4) into equation of motion (3.1) gives the standard requirement (in the limit $\hbar\to 0$) that $\mathscr{S}$ be a solution of the nonlinear partial differential equation

$$\partial\mathscr{S}(x,t)+H(x,\nabla_1\mathscr{S}(x,t),t)=0\ . \tag{3.5}$$

The Hamilton-Jacobi equation (3.5) typically has many solutions. The particular solution appropriate for (3.4) is determined by the initial condition (3.2). Recall that the free propagator [the solution of (3.1) and (3.2) in the event that $A=0$ and $v=0$] is

$$U^0(x,y;\Delta t)=\left[\frac{m}{2\pi i\hbar\Delta t}\right]^{n/2}\exp\left[\frac{i}{\hbar}\frac{m\mid x-y\mid^2}{2\Delta t}\right]. \tag{3.6}$$

The rapid oscillation and the multiplicative singularity in (3.6) become a representation of the δ function $\delta(x-y)$ in the limit $\Delta t\to 0$. We look for a similar behavior to develop in (3.4) as $\Delta t\to 0$.

Defined by the Lagrangian (2.1) and the two-fixed-end-point classical paths $q(\tau)\equiv q(\tau;x,t;y,s)$ discussed in Sec. II; the action

$$S(x,t;y,s)=\int_s^t L(q(\tau),\dot q(\tau),\tau)d\tau \tag{3.7}$$

is a known[67] solution of (3.5). Further, if the $\Delta t\to 0$ limit of (3.7) is examined it is found without difficulty that

$$\begin{aligned}S(x,t;y,s)=&\frac{m\mid x-y\mid^2}{2\Delta t}\\&+(x-y)\cdot\int_0^1 A(\hat\xi,s)d\xi+O(\Delta t)\ .\end{aligned} \tag{3.8}$$

Thus S is a singular solution (as $\Delta t\to 0$) of the Hamilton-Jacobi equation such that its leading singular term exactly reproduces the rapidly oscillating phase factor required for the δ-function representation (3.6). So choosing

$$\mathscr{S}(x,t)=S(x,t;y,s) \tag{3.9}$$

allows (3.4) to satisfy the initial condition (3.2) provided that

$$\Psi(y,s;y,s)=0\ . \tag{3.10}$$

The final step in specifying the generalized WKB approximation is to determine the function $\Psi(x,t;y,s)$. This is done by calculating the coefficients ψ_p in the series representation of Ψ, namely

$$\Psi=\sum_{p=1}^{\infty}(i\hbar)^{p-1}\psi_p\ . \tag{3.11}$$

The differential equation satisfied by Ψ is obtained by substituting (3.4) into (3.1) and using (3.5). One finds that

$$\left[\frac{\partial}{\partial t}+\left[\frac{x-y}{\Delta t}-\frac{1}{m}A(x,t)\right]\cdot\nabla_x\right]\Psi(x,t;y,s)=\frac{1}{2m}[i\hbar\mid\nabla_1\Psi\mid^2+2\nabla_1\Psi\cdot\nabla_1\psi_0+\Delta_1(i\hbar\Psi+\psi_0)+\nabla\cdot A]\ , \tag{3.12}$$

where ψ_0 is defined by

$$\psi_0(x,t;y,s)\equiv\frac{m}{2}\frac{\mid x-y\mid^2}{\Delta t}-S(x,t;y,s) \tag{3.13}$$

and the omitted arguments are the same as their last appearance. From (3.8) it is seen that ψ_0 is nonsingular as $\Delta t\to 0$.

Inserting series (3.11) into (3.12) gives, upon equating the coefficients of common powers of $\hbar$

$$\left[\frac{\partial}{\partial t}+\left[\frac{x-y}{\Delta t}-\frac{1}{m}\nabla_1\psi_0-\frac{1}{m}A\right]\cdot\nabla_x\right]\psi_p=\frac{1}{2m}\delta_{p,1}\nabla\cdot A+\frac{1}{2m}\Delta_1\psi_{p-1}+\frac{1}{2m}\sum_{k=1}^{p-1}\nabla_1\psi_{p-k}\cdot\nabla_1\psi_k\ , \tag{3.14}$$

where $p\geq 1$, $\delta_{p,1}$ is the Kronecker delta, and the sum is absent if $p=1$. The condition (3.10) requires that (3.14) be solved subject to the boundary condition

$$\psi_p(y,s;y,s)=0,\quad p\geq 1\ . \tag{3.15}$$

The transport method for solving (3.14) is based on the observation that an appropriate variable substitution will alter (3.14) from a first-order partial differential equation in $n+1$ variables to a first-order ordinary differential equation.

Using (3.13) to replace ψ_0 yields

$$\partial_1\psi_p+\frac{1}{m}(\nabla_1 S-A)\cdot\nabla_1\psi_p=\frac{1}{2m}\left[\delta_{p,1}\nabla\cdot A+\Delta_1\psi_{p-1}+\sum_{k=1}^{p-1}\nabla_1\psi_{p-k}\cdot\nabla_1\psi_k\right]\ . \tag{3.16}$$

In this identity replace $x=q(\tau)$ and $t=\tau$ where $s\leq\tau\leq t$. Now recall[67] that the gradient on the first vector argument of S with the appropriate path arguments is the momentum conjugate to $q(\tau)$

$$\nabla_1 S(q(\tau),\tau;y,s)=p(\tau)=m\dot q(\tau)+A(q(\tau),\tau)\ ,$$

where the second equality is (2.2a). With this substitution the left-hand side of (3.16) becomes a total derivative in the τ variable

$$\frac{d}{d\tau}\psi_p(q(\tau),\tau;y,s)\ ,$$

and so (3.16) is now an ordinary differential equation that may be solved by integrating with respect to τ. The one constant of integration is fixed by condition (3.15). In this way ψ_p $(p\geq 1)$ is expressed as a functional of q:

$$\psi_p(x,t;y,s)=\frac{1}{2m}\int_s^t d\tau\left[\delta_{p,1}\nabla\cdot A(q(\tau),\tau)+\left[\Delta_1\psi_{p-1}+\sum_{k=1}^{p-1}\nabla_1\psi_{p-k}\cdot\nabla_1\psi_k\right](q(\tau),\tau;y,s)\right]\ . \tag{3.17}$$

Since the right-hand side of (3.17) only involves $\psi_0\sim\psi_{p-1}$, it may be used in conjunction with knowledge of the path q, to determine ψ_p in a recursive fashion. Representation (3.17) is the main result of the transport method.

A few comments about our representation of the WKB approximation (3.4) are in order. Often in the literature one encounters a different version of the lowest-order WKB expansion,[11,23,24,31] namely

$$\langle x\mid U(t,s)\mid y\rangle\sim\frac{1}{(2\pi i\hbar)^{n/2}}\mid D(x,t;y,s)\mid^{1/2}e^{(i/\hbar)S(x,t;y,s)}\ , \tag{3.18}$$

where

$$D(x,t;y,s)=\det[-\nabla_1^\alpha\nabla_2^\beta S(x,t;y,s)]\ .$$

The determinant D may be interpreted as the density of paths from y to x, and of course becomes singular if $q(\tau)$ encounters a caustic. However, the identity

$$D(x,t;y,s)=\left[\frac{m}{t-s}\right]^n\exp\left[\frac{1}{m}\int_s^t d\tau[\nabla\cdot A(q(\tau),\tau)+\Delta_1\psi_0(q(\tau),\tau;y,s)]\right] \tag{3.19}$$

establishes that the first-order version of (3.4) with Ψ replaced by ψ_1 is identical with (3.18). Identity (3.19) is a consequence of the continuity equation[8,39] obeyed by D, and is proved in Ref. 68 in the case where $A=0$; the argument given there readily generalizes to the $A\neq 0$ case.

The gauge-transformation properties of the propagator are useful in understanding the structure and interpretation of the higher coefficients ψ_j appearing in the WKB approximation. Consider an arbitrary gauge transformation $(\mathscr{A},\phi)\to(\tilde{\mathscr{A}},\tilde\phi)$ induced by a smooth function λ: $\mathbb{R}^4\to\mathbb{R}$. The corresponding gauge transformation for the $n+1$ dimensional potentials is

$$\tilde A(x,t)=A(x,t)+\nabla\Lambda(x,t)\ , \tag{3.20a}$$

$$\tilde v(x,t)=v(x,t)-\partial\Lambda(x,t)\ , \tag{3.20b}$$

where in the notation of Sec. II,

$$\Lambda(x,t)\equiv\sum_{i=1}^N Q_i\lambda(\mu_i^{-1/2}r^i,t)\ .$$

First note that the tensor $F_{\alpha\beta}$ and the force vector f_α are invariant under the gauge transformation. From Newton's equation of motion (2.3) it follows that the classical path $q(\tau)$ is also invariant. The gauge-transformed Lagrangian (2.1) is

$$\tilde L(x,\dot x,t)=\frac{m}{2}\dot x^2+\tilde A(x,t)\cdot\dot x-\tilde v(x,t)\ .$$

Using these facts it is an elementary calculation to determine that the induced change of the action (or equivalently ψ_0) is

$$\tilde{S}(x,t;y,s)-S(x,t;y,s)=-\tilde{\psi}_0(x,t;y,s)+\psi_0(x,t;y,s)=\Lambda(x,t)-\Lambda(y,s)\ . \tag{3.21}$$

The gauge transformation behavior of the remaining coefficient functions ψ_p ($p\geq 1$) is given by (3.17). If $p=1$, there are canceling contributions from the $\nabla\cdot A$ and $\Delta_1\psi_0$ terms that leave ψ_1 invariant. For $p\geq 2$, only the invariant quantities $\psi_1\sim\psi_{p-1}$ appear in the functional relationship (3.17). Thus only the coefficient ψ_0 has a gauge dependence, which is that found in Eq. (3.21). Further note that the right-hand side of (3.21) is independent of mass, so we may conclude that the entire gauge dependence of the propagator is confined to the mass-independent part of the phase in (3.4).

IV. THE WIGNER-KIRKWOOD EXPANSION

A complete account of the large-mass expansion of the propagator is arrived at by combining the reciprocal-mass expansion of the classical path $q(\tau)$ given in Sec. II together with the transport functional identities (3.17) for ψ_p. The WK approximation has the general form (as $m\to\infty$)

$$\langle x\mid U(t,s)\mid y\rangle\sim U^0(x,y;\Delta t)\exp\left[\frac{1}{i\hbar}\left[\Delta t\int_0^1 d\xi v(\tilde{\xi})-(x-y)\cdot\int_0^1 d\xi\, A(\tilde{\xi})\right]\right]\exp\left[\frac{1}{m}J_1+\frac{1}{m^2}J_2+\frac{1}{m^3}J_3+\cdots\right], \tag{4.1}$$

where the coefficients J_p depend on $\hbar$ but not m. In this section (4.1) will be derived as a consequence of the $m\to\infty$ limit of the WKB approximation

$$\langle x\mid U(t,s)\mid y\rangle\sim\left[\frac{m}{2\pi i\hbar\Delta t}\right]^{n/2}\exp\left[\frac{i}{\hbar}S(x,t;y,s)+\psi_1+i\hbar\psi_2+(i\hbar)^2\psi_3+\cdots\right]. \tag{4.2}$$

In particular we will determine the diagonal ($x=y$) and the off-diagonal ($x\neq y$) expressions for the coefficients J_p. The structure of the WK approximation given in (4.1) is slightly different from that stated in (1.8) for the static scalar case. However, a cumulant expansion of the last exponential factor in (4.1) leads to the result quoted in (1.8). It is evident from (3.3) that when a vector potential A is present, the time evolution kernel will not depend on $\hbar$ and m only through the combination $\hbar^2/2m$.

Consider first the expansion of the action S (or equivalently ψ_0) in inverse powers of m. From (2.7)—(2.9) and (3.7) it follows that

$$\psi_0=\sum_{k=0}^{\infty}m^{-k}G_0^k\ , \tag{4.3}$$

where G_0^k are m and $\hbar$ independent coefficients. If (4.3) is used in (3.17) in conjunction with the m^{-1} expansion of $q(\tau)$ one can again obtain a large-mass series expansion for ψ_1. Upon iterating this procedure all ψ_p are seen to have an m^{-1} expansion. The explicit mass factor appearing in (3.17) means that the least m^{-1} power in ψ_p is m^{-p}, so

$$\psi_p=\sum_{k=p}^{\infty}m^{-k}G_p^k\ . \tag{4.4}$$

Of particular importance is the coefficient G_0^0. We begin with ψ_0; here (2.6), (2.7), and (3.9) lead to

$$\psi_0(x,t;y,s)=\frac{m\mid x-y\mid^2}{2\Delta t}-\int_s^t d\tau\left[\frac{m}{2}\mid\dot{\rho}_0+\dot{\eta}(\tau)\mid^2+A(q(\tau),\tau)\cdot\dot{q}(\tau)-v(q(\tau),\tau)\right].$$

Recall $\dot{\rho}_0=(x-y)/\Delta t$ is constant. The quadratic velocity term in the integrand gives rise to three terms: One cancels the leading term above; the cross term integrates and vanishes due to (2.8); if the third term is integrated by parts there are no end-point contributions due to (2.8). Since $\ddot{\eta}=\ddot{q}$, (2.3) yields

$$\begin{aligned}\psi_0&=\int_s^t d\tau\{\tfrac{1}{2}\eta_\alpha(\tau)[f_\alpha(q(\tau),\tau)+\dot{q}_\beta(\tau)F_{\alpha\beta}(q(\tau),\tau)]-\dot{q}(\tau)\cdot A(q(\tau),\tau)+v(q(\tau),\tau)\}\\&=\int_s^t d\tau[\tfrac{1}{2}\eta_\alpha(\tau)e^{\eta(\tau)\cdot\nabla}f_\alpha(\rho_0(\tau),\tau)+\tfrac{1}{2}\eta_\alpha(\tau)\dot{q}_\beta(\tau)e^{\eta(\tau)\cdot\nabla}F_{\alpha\beta}(\rho_0(\tau),\tau)\\&\qquad-\dot{q}_\alpha(\tau)e^{\eta(\tau)\cdot\nabla}A_\alpha(\rho_0(\tau),\tau)+e^{\eta(\tau)\cdot\nabla}v(\rho_0(\tau),\tau)]\ .\end{aligned} \tag{4.5}$$

For the sake of brevity, we adopt the following notational conventions. If the argument of a ψ or G is omitted, it is to be taken as $(x,t;y,s)$. Similarly for the fields A,v,f,F omitted arguments are to be $(\rho_0(\tau),\tau)$, and for the path variables q,ρ,η we will omit (τ). The evaluation of any such quantity at a different argument will be made explicit.

Collecting the parts of ψ_0 proportional to m^{-0} shows that

$$G_0^0=\int_s^t d\tau[-\dot{\rho}_{0\alpha}A_\alpha(\rho_0,\tau)+v(\rho_0,\tau)]\ . \tag{4.6}$$

Changing variables to the unit interval, $\tau=s+\xi\Delta t$, the arguments of A_α and v become $\tilde{\xi}$ [cf. (2.16)] so that G_0^0 may be expressed as the linear path parametric integral ($I \equiv [0,1]$):

$$G_0^0(x,t;y,s)=\Delta t \int_I d\xi \left[v(\tilde{\xi}) - \frac{x-y}{\Delta t}\cdot A(\tilde{\xi}) \right] . \quad (4.7)$$

This term completely provides for the change of ψ_0 under a gauge transformation, and gives the first exponential factor in the WK representation (4.1). In fact comparing (4.1) with (4.2) and utilizing (4.3) and (4.4) requires

$$J_p = \sum_{l=0}^{p} (i\hbar)^{l-1} G_l^p . \quad (4.8)$$

We shall illustrate the calculation of J_p by determining this coefficient for $p=1,2$. From (4.8) it is seen that we need to find G_0^1, G_1^1 for J_1 and G_0^2, G_1^2, and G_2^2 for J_2. First, consider G_0^1. Return to (4.5), after using (2.12) to collect the m^{-1} terms. One finds

$$G_0^1 = \int_s^t d\tau [\tfrac{1}{2}\rho_{1\alpha} f_\alpha + \tfrac{1}{2}\rho_{1\alpha}\dot{\rho}_{0\beta}F_{\alpha\beta} - \dot{\rho}_{0\alpha}(\rho_1\cdot\nabla)A_\alpha - \dot{\rho}_{1\alpha}A_\alpha + (\rho_1\cdot\nabla)v] .$$

Integrate by parts the $\dot{\rho}_{1\alpha}A_\alpha$ term; noting (2.10) and that

$$\frac{d}{d\tau}A_\alpha(\rho_0,\tau) = \nabla^\beta A_\alpha(\rho_0,\tau)\dot{\rho}_{0\beta} + \partial A_\alpha(\rho_0,\tau) ,$$

we obtain the gauge-invariant form

$$G_0^1 = -\tfrac{1}{2}\int_s^t d\tau \rho_{1\alpha}(f_\alpha + \dot{\rho}_{0\beta}F_{\alpha\beta}) .$$

Changing variables to the unit interval and using (2.18) yields the final expression

$$G_0^1(x,t;y,s) = \tfrac{1}{2}(\Delta t)^3 \int_{I^2} d^2\xi\, g(\xi_1,\xi_2)\omega_\alpha(\tilde{\xi}_1)\omega_\alpha(\tilde{\xi}_2) . \quad (4.9)$$

Now turn to G_1^1. Set $p=1$ in (3.17) and collect the m^{-1} parts of the resulting formula to obtain

$$G_1^1 = \tfrac{1}{2}\Delta t \int_I d\xi [\nabla\cdot A(\tilde{\xi}) + \Delta_1 G_0^0(\tilde{\xi};y,s)] . \quad (4.10)$$

Recall that G_1^1 is gauge invariant, but that A and G_0^0 are not. Hence, it is desirable to have a simple method for canceling $\nabla\cdot A$ with part of $\Delta_1 G_0^0$ in (4.10) so as to leave a manifestly gauge-invariant result. This method, which is useful for all G_1^j ($j\geq 1$), works as follows. Differentiate (4.7) with respect to x_α, remembering the x dependence in $\tilde{\xi}$,

$$\nabla_1^\alpha G_0^0 = \int_I d\xi [\xi\Delta t \nabla^\alpha v(\tilde{\xi}) - \xi(x-y)_\beta \nabla^\alpha A_\beta(\tilde{\xi}) - A_\alpha(\tilde{\xi})] .$$

The last term is integrated by parts

$$-\int_0^1 d\xi \left[\frac{d}{d\xi}\xi\right] A_\alpha(\tilde{\xi}) = -A_\alpha(x,t) + \int_0^1 d\xi\, \xi[(x-y)_\beta \nabla^\beta A_\alpha(\tilde{\xi}) + \Delta t\, \partial A_\alpha(\tilde{\xi})] ,$$

resulting in the useful formula

$$\nabla_1^\alpha G_0^0(x,t;y,s) = -A_\alpha(x,t) - C_\alpha(x,t;y,s) ,$$

where C is manifestly gauge invariant,

$$C_\alpha(x,t;y,s) \equiv \Delta t \int_I d\lambda\, \lambda\omega_\alpha(\tilde{\lambda}) . \quad (4.11)$$

Hence the Laplacian of G_0^0 with respect to its first argument is

$$\Delta_1 G_0^0 = -\nabla\cdot A(x,t) - \nabla_1\cdot C .$$

Substituting this result into (4.10), wherein the (x,t) is replaced by $\tilde{\xi}$ we find the $\nabla\cdot A$ terms cancel leaving

$$G_1^1 = -\tfrac{1}{2}\Delta t \int_I d\xi\, \nabla_1\cdot C(\tilde{\xi};y,s) .$$

Now (4.11) gives

$$\nabla_1\cdot C \equiv \frac{d}{dx_\alpha} C_\alpha(x,t;y,s)$$

$$= \Delta t \int_I d\lambda\, \lambda \left[\lambda\nabla^\alpha f_\alpha(\tilde{\lambda}) + \lambda\frac{(x-y)_\beta}{\Delta t}\nabla^\alpha F_{\alpha\beta}(\tilde{\lambda}) + \frac{1}{\Delta t}F_{\alpha\alpha}(\tilde{\lambda}) \right]$$

$$= \Delta t \int_I d\lambda\, \lambda^2 \nabla\cdot\omega(\tilde{\lambda})$$

by the antisymmetry of $F_{\alpha\beta}$. Recalling (2.18) gives

$$G_1^1 = -\tfrac{1}{2}\Delta t \int_0^1 d\xi\, \xi\Delta t \int_0^1 d\lambda\, \lambda^2 \nabla\cdot\omega(\tilde{\gamma})$$

where $\gamma = \lambda\xi$. Finally, make the change of variables $\gamma=\lambda\xi$ in the inner integral and follow that by a change of order of integration. The ξ integral over $[\gamma,1]$ may be exactly evaluated and the result is

$$G_1^1(x,t;y,s) = -\tfrac{1}{2}(\Delta t)^2 \int_I d\gamma\, \gamma(1-\gamma)\nabla\cdot\omega(\tilde{\gamma}) . \quad (4.12)$$

Together formulas (4.9) and (4.12) sum via (4.8) to give J_1.

The coefficient J_2 requires the construction of G_0^2, G_1^2, and G_2^2. Consider G_2^2 first. Using the fact that ψ_j begins with $m^{-j}G_j^j$ we see that the transport identity implies that for $p\geq 1$

$$G_p^p = \tfrac{1}{2}\Delta t \int_I d\xi\, \Delta_1 G_{p-1}^{p-1}(\tilde{\xi};y,s) . \quad (4.13)$$

Upon inserting expression (4.12) for G_1^1 and iterating (4.13) we obtain the general result for all $p\geq 1$

$$G_p^p(x,t;y,s) = -(2^p p!)^{-1}(\Delta t)^{p+1} \times \int_I d\xi [\xi(1-\xi)]^p (\Delta)^{p-1}\nabla\cdot\omega(\tilde{\xi}) .$$

It remains to obtain G_0^2 and G_1^2. The m^{-2} parts of (4.5) give G_0^2. Proceeding as in the calculation of G_0^1 and upon implementing an integration by parts to bring the expressions into a manifestly gauge-invariant form we find

$$G_0^2(x,t;y,s)=-\tfrac{1}{2}(\Delta t)^5\int_{I^3}d^3\xi\, g(\xi_1,\xi_2)\omega_\alpha(\tilde{\xi}_1)\omega_\beta(\tilde{\xi}_3)[g(\xi_2,\xi_3)\nabla^\beta\omega_\alpha(\tilde{\xi}_2)+(\Delta t)^{-1}\partial_1 g(\xi_2,\xi_3)F_{\alpha\beta}(\tilde{\xi}_2)]\ . \tag{4.14}$$

Finally the m^{-2} parts of (3.17) with $p=1$ give G_1^2. The resulting formula is

$$\begin{aligned}G_1^2=\tfrac{1}{4}(\Delta t)^4\int_{I^2}d^2\xi\, g(\xi_1,\xi_2)\{&g(\xi_1,\xi_2)[\nabla^\alpha\omega_\beta(\tilde{\xi}_1)+(\xi_1\Delta t)^{-1}F_{\beta\alpha}(\tilde{\xi}_1)][\nabla^\alpha\omega_\beta(\tilde{\xi}_2)+(\xi_2\Delta t)^{-1}F_{\beta\alpha}(\tilde{\xi}_2)]\\&+\xi_2^2\xi_>^{-1}(1-\xi_>)\omega_\beta(\tilde{\xi}_1)[\Delta\omega_\beta(\tilde{\xi}_2)+2(\xi_2\Delta t)^{-1}\nabla^\alpha F_{\beta\alpha}(\tilde{\xi}_2)]\\&+\xi_2\xi_>^{-1}[2\xi_>-(\xi_>+1)\xi_2]\omega_\beta(\tilde{\xi}_1)[\nabla^\beta\nabla^\alpha\omega_\alpha(\tilde{\xi}_2)+(\xi_2\Delta t)^{-1}\nabla^\alpha F_{\alpha\beta}(\tilde{\xi}_2)]\}\end{aligned} \tag{4.15}$$

where $\xi_>=\max\{\xi_1,\xi_2\}$.

In a number of physical applications it suffices to know the trace of the propagator in $\mathscr{H}$. The trace is the dx integral of the diagonal values of WK expansion formulas. In the case of a static field ($\partial v=\partial A_\alpha=0$) there is a substantial simplification of the general expansion coefficients. The diagonal values of the relevant G_l^p are

$$G_0^1(x,t;x,s)=\tfrac{1}{24}(\Delta t)^3\,|\nabla v(x)|^2\ ,$$

$$G_0^2(x,t;x,s)=\frac{1}{2}\frac{1}{5!}(\Delta t)^5\nabla^\beta v(x)\nabla^\alpha v(x)\nabla^\beta\nabla^\alpha v(x)\ ,$$

$$G_p^p(x,t;x,s)=\frac{2^{-p}p!}{(2p+1)!}(\Delta t)^{p+1}\Delta^p v(x),\quad p\geq 0\ ,$$

and

$$G_1^2(x,t;x,s)=\tfrac{1}{48}(\Delta t)^2F_{\beta\alpha}(x)F_{\beta\alpha}(x)+(\Delta t)^4\left[\frac{2}{6!}\nabla^\alpha\nabla^\beta v(x)\nabla^\alpha\nabla^\beta v(x)+\frac{1}{5!}\nabla^\beta v(x)\nabla^\beta\Delta v(x)\right]\ .$$

In the G_l^p above, the static magnetic field only appears in the term G_1^2, whereas the static electric field appears in all the terms. By contrast all the G_l^p depend (for both diagonal and off-diagonal cases) on A in the nonstatic case.

In summary, we have found that the mutual consistency and structural connection between the higher-order WKB and the higher-order WK expansion is realized by a large mass expansion. This expansion is the joint result of a large mass expansion for the classical path $q(\tau)$ and the transport recurrence identities for the correction terms that enter the WKB approximation. The structural connection just described provides a new way of deriving the generalized WK expansion. It is to be expected that this approach to the WK expansion should succeed in a wide variety of quantum problems since it only requires the weak hypothesis that the underlying classical Lagrangian be analytic in its mass parameter.

We have demonstrated these ideas by discussing in detail the case of an N-body system interacting with an external electromagnetic field. In addition to the explicit expansion formulas given in this section, it is seen that the geometrical origin of the $\xi\in[0,1]$ averages [cf. (4.14) and (4.15)], ubiquitous in the earlier treatments of the WK expansion,[6,41,46,47] lies in the $m\rightarrow\infty$ expansion of $q(\tau)$ about the linear (infinite mass) trajectory ρ_0 between y,s and x,t. Further, the weight factors $g(\xi_1,\xi_2)$, also common in these formulas, are a consequence of the two fixed end point boundary condition and Newton's equation of motion for $q(\tau)$. Illustrative of the efficiency and the ease of computation of this method is the fact that the example we have treated above subsumes all prior results in the literature (for scalar-valued wave functions) and extends the WK approximation so as to incorporate time-dependent vector and scalar potentials.

The appendix presents a second method for obtaining the large mass expansion of the propagator, which is based on recurrence relations. Although it does not convey the geometrical insight of the classical path expansion method, it is a direct and usually more practical method of computing formulas for the fundamental G_l^p coefficients.

APPENDIX: LARGE-MASS RECURRENCE RELATIONS

In Sec. IV we have determined that the functions G_l^p play the key role in constructing the WK functions J_p. There the functions G_l^p were computed using the large-mass expansion of the classical path $q(\tau)$ in combination with the transport recursion identities (3.17). However, given the form of representation (4.1)—(4.8) it is possible to obtain a recursive solution for G_l^p by a procedure which avoids the m^{-1} expansion of q entirely.

Define a complex phase function W by

$$\langle x\,|\,U(t,s)\,|\,y\rangle=U^0(x,y;\Delta t)\exp[W(x,t;y,s)]\ , \tag{A1}$$

where W depends on both $\hbar$ and m. Substituting (A1) into the Schrödinger equation (3.1) gives the nonlinear partial differential equation that W obeys,

$$\begin{aligned}\partial_1 W+\frac{x-y}{\Delta t}\cdot\nabla_1 W=&\frac{i\hbar}{2m}\,|\nabla_1 W|^2+\frac{i\hbar}{2m}\Delta_1 W-\frac{x-y}{i\hbar\Delta t}\cdot A(x,t)\\&+\frac{1}{m}A\cdot\nabla_1 W+\frac{1}{2m}\nabla\cdot A+\frac{1}{i\hbar 2m}\,|A|^2+\frac{1}{i\hbar}v(x,t)\ .\end{aligned} \tag{A2}$$

Replace $x\rightarrow\hat{\xi}=y+\xi(x-y)$ and $t\rightarrow\tau=s+\xi\Delta t$ everywhere in (A2) and then multiply by Δt,

$$\Delta t\, \partial_1 W(\tilde{\xi};y,s)+(x-y)\cdot\nabla_1 W=\frac{i\hbar}{2m}\Delta t(\,|\nabla_1 W|^2+\Delta_1 W)-\frac{1}{i\hbar}(x-y)\cdot A(\tilde{\xi})$$
$$+\frac{\Delta t}{m}A\cdot\nabla_1 W+\frac{\Delta t}{2m}\nabla\cdot A+\frac{\Delta t}{i\hbar 2m}\,|A|^2+\frac{\Delta t}{i\hbar}v(\tilde{\xi})\ . \tag{A3}$$

In the equations above, we have again employed the convention that the suppressed argument of a function is the same as the last one shown for that function. The motivation for the substitutions we have made in (A2) is that now the left-hand side of (A3) is $(d/d\xi)W(\tilde{\xi};y,s)$. This step is just a linear-path version of the transport method. The large-mass expansion of W, consistent with (4.1), is

$$W=\sum_{p=0}^{\infty} m^{-p}J_p(x,t;y,s)\ , \tag{A4}$$

where J_p depends on $\hbar$ but not on m. As $\Delta t\to 0$ the initial data condition (3.2) requires [cf. (3.8), (3.10), (3.13)] $W(y,s;y,s)=0$ or equivalently,

$$J_p(y,s;y,s)=0,\ \ p\geq 0\ . \tag{A5}$$

Inserting the expansion (A4) into (A3) and equating common powers of m^{-p} for $p\geq 0$ gives (with $J_{-1}\equiv 0$):

$$\frac{d}{d\xi}J_p(\tilde{\xi};y,s)=\tfrac{1}{2}i\hbar\Delta t\Delta_1 J_{p-1}+\tfrac{1}{2}i\hbar\Delta t\sum_{k=0}^{p-1}\nabla_1 J_{p-1-k}\cdot\nabla_1 J_k$$
$$+\Delta t A(\tilde{\xi})\cdot\nabla_1 J_{p-1}+\Delta t\frac{\delta_{p,1}}{2}\left[\nabla\cdot A+\frac{1}{i\hbar}A^2\right]+\Delta t\frac{\delta_{p,0}}{i\hbar}\left[v(\tilde{\xi})-\frac{x-y}{\Delta t}\cdot A\right]\ . \tag{A6}$$

It is a simple matter to integrate (A6) with respect to $\xi\in[0,1]$ and upon imposing (A5) find the integral equivalent of (A5) and (A6). However, we are more interested in the behavior of G_l^p. Note that boundary condition (A5) and the finite sum (4.8) expressing J_p in terms of G_l^p implies (because of the variability of $\hbar$) the condition

$$G_l^p(y,s;y,s)=0\ . \tag{A7}$$

If we substitute (4.8) into (A6), equate common powers of $\hbar$, integrate with respect to $\xi\in[0,1]$ and employ the boundary condition (A7) to determine the constant of integration, then

$$G_l^p(x,t;y,s)=\frac{\Delta t}{2}\int_0^1 d\xi\left\{\left[\Delta_1 G_{l-1}^{p-1}+\sum_{k=0}^{p-1}\ \sum_{n=\max\{0,\,l+k+1-p\}}^{\min\{k,l\}}\nabla_1 G_{l-n}^{p-1-k}\cdot\nabla_1 G_n^k+2A(\tilde{\xi})\cdot\nabla_1 G_l^{p-1}\right](\tilde{\xi};y,s)\right.$$
$$\left.+\delta_{l,1}\delta_{p,1}\nabla\cdot A(\tilde{\xi})+\delta_{l,0}\left[2\delta_{p,0}\left[v(\tilde{\xi})-\frac{x-y}{\Delta t}\cdot A(\tilde{\xi})\right]+\delta_{p,1}A(\tilde{\xi})^2\right]\right\}. \tag{A8}$$

As a check on the *a posteriori* self-consistency of the results of Sec. IV we have computed G_l^p directly from (A8). This latter method does not use in any way the large-mass expansion of the classical path $q(\tau)$. The resulting formulas for the coefficients are identical to those found in Sec. IV.

Another useful check on the coefficients G_l^p is to compare them with other results in the literature. Results of this type closely related to ours are the Wigner-Kirkwood expansions of the heat kernel $\langle x\,|\,e^{-\beta H}\,|\,y\rangle$, for time-independent Hamiltonians H, found in Refs. 41 and 55 and Ref. 6 (with and without the vector potential, respectively). By specializing our results to the static case, and replacing $\Delta t=-i\hbar\beta$ we have found the resulting G_0^0, G_0^1, G_1^1, G_2^2 to be in agreement with known results.

Using G_1^2 we have similarly verified terms 3 through 9 of Eqn. (2.29) of Ref. 55 (to use their results, one must set $T=1$ and compute some of the superfluous integrals; there are misprints in the 3rd and 8th of the above mentioned terms).

ACKNOWLEDGMENTS

A portion of the work described in this paper was carried out at the University of Maryland. The authors would like to thank the Nuclear Theory Group at Maryland for their warm hospitality. This work has been supported in part by grants from the Natural Sciences and Engineering Research Council of Canada (NSERC) and the U.S. Department of Energy. One of us (F.H.M.) gratefully acknowledges support from NSERC and the University of Manitoba.

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