Global, Uniform, Semiclassical Approximation to Wave Equations

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The usual configuration-space semiclassical approximation to wave equations (e.g., Schrödinger's equation) needs refinement at caustics. When expressed in a phase-space coherent-state representation, such equations admit a semiclassical solution that properly captures the effects of caustics. Transformation of this expression to the configuration-space representation yields a global, uniform, semiclassical approximation.

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We consider semiclassical approximations to wave equations such as the time-dependent, one-dimensional Schrödinger equation

$$i\hbar\frac{\partial\phi(x,t)}{\partial t}=\mathscr{H}\left(-i\hbar\frac{\partial}{\partial x},x\right)\phi(x,t), \quad (1)$$

where $\mathscr{H}$ denotes the operator that arises from a Weyl-ordered quantization of the classical Hamiltonian $H=H(p,q)$. Our remarks readily generalize to (i) more dimensions, (ii) time-dependent Hamiltonians, and (iii) similar wave equations as arise, for example, in the paraxial approximation to the full (hyperbolic) wave equation for a single frequency (where $\lambda\!\!\!^-$ plays the role of $\hbar$).[1]

Equation (1) admits a solution in the form

$$\phi(x'',T)=\int J(x'',T;x',0)\phi(x',0)dx' \quad (2)$$

in terms of the initial-value amplitude $\phi(x',0)$ and the propagator J for which

$$\lim_{T\to 0}J(x'',T;x',0)=\delta(x''-x'). \quad (3)$$

A path-integral representation for J readily leads to the usual semiclassical approximation, $J_{sc}\approx J$, where[2]

$$J_{sc}(x'',T;x',0)=\sum\left[\frac{-i\,\partial^2S(x'',x')}{2\pi\hbar\,\partial x''\,\partial x'}\right]^{1/2}e^{iS(x'',x')/\hbar}. \quad (4)$$

Here

$$S(x'',x')=\int_0^T[p\dot{x}-H(p,x)]dt \quad (5)$$

evaluated for a classical path that satisfies

$$\dot{x}(t)=\partial H/\partial p(t),\quad \dot{p}(t)=-\partial H/\partial x(t), \quad (6)$$

and which interpolates between $x(0)=x'$ and $x(T)=x''$. The sum runs over the several such classical paths, which are assumed to be well separated from one another. Equation (4) fails to be a good approximation when the paths are not well separated, and especially so at a caustic where paths cross. Maslov has proposed an alternative, integral representation for the right-hand side of (4) which is locally uniform but generally not globally so.[3] Recently, other alternatives have been proposed by McDonald[4] and Littlejohn.[5] Here, extending earlier work,[6] we present another semiclassical expression that provides a global, uniform approximaiton and which is applicable even when a veritable "thicket" of classical trajectories exist.

Adopting a convenient choice of phase, we introduce the coherent-state amplitude[7]

$$\psi(p,q,t)=(\pi\hbar)^{-1/4}\int\exp(-x^2/2\hbar-ipx/\hbar)\phi(x+q,t)dx, \quad (7)$$

and the inverse transformation

$$\phi(q,t)=\frac{(\pi\hbar)^{1/4}}{2\pi\hbar}\int\psi(p,q,t)dp, \quad (8)$$

which have been normalized so that

$$\int|\phi(x,t)|^2dx=\int|\psi(p,q,t)|^2(dp\,dq/2\pi\hbar). \quad (9)$$

It follows directly that (1) is replaced by

$$i\hbar\partial\psi(p,q,t)/\partial t=\mathscr{H}(-i\hbar\,\partial/\partial q,q+i\hbar\,\partial/\partial p)\psi(p,q,t), \quad (10)$$

which admits a solution in the form

$$\psi(p'',q'',T)=\int K(p'',q''T;p',q',0)\psi(p',q',0)(dp'\,dq'/2\pi\hbar) \quad (11)$$

in terms of the initial-value amplitude and the coherent-state propagator K. The smoothness of every ψ implies that they do not span all of $L^2(\mathscr{R}^2)$ but rather are members of a proper subspace which is a reproducing-kernel Hilbert space.[7] Consequently it is appropriate to choose

$$\lim_{T\to 0} K(p'',q'',T;p',q',0) = \exp(\hbar^{-1}\{\tfrac{1}{2}i(p''+p')(q''-q') - \tfrac{1}{4}[(p''-p')^2+(q''-q')^2]\}), \tag{12}$$

which is the reproducing kernel itself. With this choice it follows that $|K| \leq 1$ uniformly.

Recently a representation of K was given for a wide class of Hamiltonians as the limit of well-defined path integrals over pinned Brownian p and q paths in the limit that the diffusion constant diverges.[8] In a formal way this representation may be given as

$$K(p'',q'',T;p',q',0) = \lim_{\nu\to\infty} \mathscr{M}\int \exp\{(i/\hbar)\int[p\dot{q} - h(p,q)]dt - (1/2\hbar\nu)\int[\dot{p}^2+\dot{q}^2]dt\}\prod_t dp(t)\,dq(t),$$

$$h(p,q) = \exp[-(\hbar/4)(\partial_p^2+\partial_q^2)]H(p,q). \tag{13}$$

This phase-space path integral may, in turn, be approximately evaluated by stationary-phase methods leading to a semiclassical solution, $K_{\text{sc}} \approx K$, where

$$K_{\text{sc}}(p'',q'',T;p',q',0) = AK_{\text{sc}}^0(p'',q'',T;p',q',0), \quad K_{\text{sc}}^0(p'',q'',T;p',q',0) = \exp[iF(p'',q'';p',q')/\hbar],$$

$$A = [\tilde{p}(T) + i\tilde{q}(T)]^{-1/2}. \tag{14}$$

Solution of the extremal equations that follow from (13), and an evaluation of the quadratic fluctuations, lead, as $\nu \to \infty$, to the factors which appear in (14). Specifically,

$$F = \tfrac{1}{2}(p''q''-p'q') + \tfrac{1}{2}(p''\bar{q}''-q''\bar{p}''-\bar{q}'p'+\bar{p}'q') + \int[\tfrac{1}{2}(\bar{p}\dot{\bar{q}}-\bar{q}\dot{\bar{p}}) - H(\bar{p},\bar{q})]dt, \tag{15}$$

where $\bar{P}(t),\bar{q}(t)$ [with $\bar{p}'=\bar{p}(0)$, $\bar{q}'=\bar{q}(0)$, $\bar{p}''=\bar{p}(T)$, and $\bar{q}''=\bar{q}(T)$], denotes a generally *complex* solution of the analytically continued classical equations of motion,

$$\dot{\bar{q}} = \partial H/\partial\bar{p}(t), \quad \dot{\bar{p}}(t) = -\partial H/\partial\bar{q}(t), \tag{16}$$

subject to the boundary conditions $q'+ip' = \bar{q}'+i\bar{p}'$, $\bar{q}''-i\bar{p}'' = q''-ip''$. To find a solution to these equations set $\bar{q}' = q'+w$ and $\bar{p}' = p'+iw$ and choose the free complex parameter w to satisfy the final boundary condition; the proper solution is continuous for all $T \geq 0$. The amplitude factor A is determined as the solution of the linearized, classical Hamiltonian system of equations

$$\dot{\tilde{p}}(t) = -\beta(t)\tilde{p}(t) - \gamma(t)\tilde{q}(t), \quad \dot{\tilde{q}}(t) = \alpha(t)\tilde{p}(t) + \beta(t)\tilde{q}(t), \tag{17}$$

subject to the initial condition $\tilde{p}(0) = 1/2$, $\tilde{q}(0) = -i/2$, where

$$\alpha(t) = \partial_{\bar{p}}^2 H(\bar{p},\bar{q}), \quad \beta(t) = \partial_{\bar{p}}\partial_{\bar{q}}H(\bar{p},\bar{q}), \quad \gamma(t) = \partial_{\bar{q}}^2 H(\bar{p},\bar{q}), \tag{18}$$

evaluated for the extremal trajectory.

In the analysis of (14) it is useful to distinguish two types of paths. In the special case that the classical evolution of the phase point (p',q') in time T with the classical Hamiltonian H *coincides* with (p'',q''), then $w=0$, F is real, and $|K_{\text{sc}}^0| = 1$. More generally, $w \neq 0$, F is complex, and importantly in that case it follows that $|K_{\text{sc}}^0| < 1$, which for small $\hbar$ leads to an *exponential* reduction in the amplitude of K_{sc}^0. The subdominant factor A is, in Dirac notation, alternatively given by

$$A = \langle 0|\mathscr{T}\exp[-(i/\hbar)\int\mathscr{H}_2(t)dt]|0\rangle, \quad \mathscr{H}_2(t) = \tfrac{1}{2}[\alpha(t)P^2 + \beta(t)(PQ+QP) + \gamma(t)Q^2], \tag{19}$$

where $\mathscr{T}$ denotes time ordering, $[Q,P] = i\hbar$, and $|0\rangle$ is the normalized oscillator ground state with $(q+iP)|0\rangle = 0$. Stability requires that $\mathscr{H}_2$ be dissipative, i.e., $i(\mathscr{H}_2 - \mathscr{H}_2^\dagger) \geq 0$, and thus it follows that $|A| \leq 1$. In particular, if $\beta = 0$, $\alpha = \gamma$, and $\text{Im}\alpha = 0$, then $A = \exp[-\tfrac{1}{2}i\int\alpha(t)dt]$; even this phase factor can be eliminated from such a quadratic Hamiltonian by normal ordering.[6,9]

The required global, uniform, semiclassical approximation follows from K_{sc} and is given by

$$\tilde{J}_{\text{sc}}(q'',T;q',0) = \frac{(\pi\hbar)^{1/2}}{(2\pi\hbar)^2}\int K_{\text{sc}}(p'',q'',T;p',q',0)\,dp''\,dp'. \tag{20}$$

It is of interest to see how the expected properties of $\tilde{J}_{sc}$ arise in such a double integral. Normally the integrand of (20) is exponentially small *except* at those several special pairs $p'=p_c'$ and $p''=p_c''$ that correspond to genuine classical trajectories beginning with (p',q') and ending at (p'',q'') in time T with Hamiltonian H. Each of these classical trajectories will contribute with a weight roughly determined by how fast K_{sc}^0 decreases in amplitude and changes phase near (p_c',p_c''). Such an evaluation automatically gives the proper contribution for various caustics, or even when the classical paths are not well separated for a finite interval (a "thicket"). Moreover, if some component of the Hamiltonian is a normal stochastic variable, then an ensemble average of powers of the K propagator and its complex conjugate lead to a multipath path integral that can be approximated as described here provided the Markov approximation is adopted for the correlation function.[10]

Under suitable conditions the integrals in (20) may themselves be carried out by a stationary-phase approximation.[9] Near each isolated classical trajectory we set

$$F=F(p_c''+(p''-p_c''),q'';p_c'+(p'-p_c'),q') \quad (21)$$

and expand F out to linear and quadratic terms in $p''-p_c''$ and $p'-p_c'$. Integration over p'' and p' can then be carried out analytically yielding a suitable approximation save in the case that the matrix of quadratic deviations is degenerate. In that case at least one term cubic in the deviations is required leading to the expected Airy function. In more-dimensional cases what counts is the behavior of F in the vicinity of the special phase-space points where F is real. Deviations therefrom may be catalogued as to type on the basis of the classification scheme of catastrophe theory. In each case the dependence on $\hbar$ can be scaled out and the resultant integral numerically evaluated. Indeed, for this aspect of the work one may draw on similar studies in configuration-space approaches.[2,11] The final behavior is obtained by the assembly of the appropriate contributions for the problem at hand. The result is, as it must be, qualitatively similar to that of more conventional approaches. However, since the result will typically differ in detail there is the prospect for an improved semiclassical approximation.

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