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Annals of Physics 323 (2008) 654–672

ANNALS of PHYSICS

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Controlling phase space caustics in the semiclassical coherent state propagator

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Received 22 March 2007; accepted 4 April 2007
Available online 12 April 2007

Abstract

The semiclassical formula for the quantum propagator in the coherent state representation $\langle \mathbf{z}''|e^{-i\hat{H}T/\hbar}|\mathbf{z}'\rangle$ is not free from the problem of caustics. These are singular points along the complex classical trajectories specified by $\mathbf{z}'$, $\mathbf{z}''$ and T where the usual quadratic approximation fails, leading to divergences in the semiclassical formula. In this paper, we derive third order approximations for this propagator that remain finite in the vicinity of caustics. We use Maslov's method and the dual representation proposed in Phys. Rev. Lett. 95, 050405 (2005) to derive uniform, regular and transitional semiclassical approximations for coherent state propagator in systems with two degrees of freedom.

PACS: 02.30.Mv; 03.65.Sq; 31.15.Gy

Keywords: Semiclassical methods; Quantum chaos; Coherent states

1. Introduction

Semiclassical methods are the fundamental tool in the study of the quantum-classical connection. In the limit where typical actions S become much larger than Planck's constant $\hbar$, it is possible to use classical ingredients, usually classical trajectories, to produce

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0003-4916/$ - see front matter
doi:10.1016/j.aop.2007.04.008

approximations to quantum mechanical objects, like matrix elements, wavefunctions and propagators. In Feynman's path integral approach to quantum mechanics, semiclassical approximations consist in realizing that the classical paths become dominant as $S \gg \hbar$ and it suffices to add together the contributions of a small set of neighboring paths in the vicinity of the classical one. This apparently simple procedure, however, has two well known caveats that make the application of such formulas difficult: the existence of non-contributing classical solutions and the presence of focal points or caustics.

The first of these issues, which is not going to be further discussed in this paper, is closely related to the *Stokes Phenomenon*, which is the abrupt change in the number of contributing solutions to an asymptotic formula when a certain boundary in parameter space is crossed [1–3]. Although a general criterion to decide whether a trajectory should be included or not as a true contribution to the formula exists, it is usually hard to verify in practice. An example of a careful study of these solutions can be found in [4]. More generally, one resorts to a simple *a posteriori* criterion: the contribution of each trajectory is computed and, if it leads to non-physical results, it is discarded. This kind of prescription has been widely used in the last years as, for example, in the semiclassical formula of the coherent state propagator in one [5] and two [6] spatial dimensions, in the momentum propagator [7] and in the semiclassical evolution of gaussian wave packets [8].

Singularities due to caustics are the other recurrent problem in semiclassical formulas. In the WKB theory [9] the semiclassical wavefunction in the position representation diverges at the turning points $\dot{q} = 0$. In the momentum representation the equivalent problem occurs at the points where $\dot{p} = 0$. In addition, for the Van-Vleck propagator, which is a semiclassical formula of the propagator in the coordinate representation, $\langle q'' | e^{-i\hat{H}T/\hbar} | q' \rangle$, singularities occur at the focal points [10]. These are points along the trajectory from $q(0) = q'$ to $q(T) = q''$ where an initial set of trajectories issuing from the same initial point $q(0)$ but with slightly different momenta, get together again, focusing at the same point $q(t)$.

The failure of the semiclassical approximation at these points, and the reason why a singularity develops there, is that the usual quadratic approximation used to derive such formulas becomes degenerate and third order contributions around the stationary points become essential. The standard procedure to obtain improved formulas valid at caustics is due to Maslov [11] and it consists in changing to a dual representation where the singularity does not exist [11,12]. For a singularity in coordinates, one uses the momentum representation and vice-versa. The trick is that, when transforming back to the representation where the singularity exists, one should go beyond the quadratic approximation, otherwise the singularity re-appears.

The subject of the present paper is the treatment of singularities due to caustics in the semiclassical formula of the coherent state propagator in two spatial dimensions $K(\mathbf{z}''^*, \mathbf{z}', T) \equiv \langle \mathbf{z}'' | e^{-i\hat{H}T/\hbar} | \mathbf{z}' \rangle$. In spite of the fact that this is a phase space representation, where no turning points exist, this propagator is not free from caustics [5,6,13,14], although earlier works on the subject indicated so [15–18]. These points have been termed *phase space caustics*.

The caustics in $K_{SC}(\mathbf{z}''^*, \mathbf{z}', T)$ have the same origin as the focal point divergence in the Van-Vleck propagator, namely, the breakdown of the quadratic approximation. Therefore, it is natural to look for a dual representation as in Maslov's method to derive higher order approximations. However, since both coordinates and momenta are used in the coherent states, there seems to be no room for a natural dual representation. In a recent