Annals of Physics 371 (2016) 437–459

Contents lists available at ScienceDirect

Annals of Physics

journal homepage: www.elsevier.com/locate/aop

Trajectory description of the quantum–classical transition for wave packet interference

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ARTICLE INFO

Article history:
Received 26 April 2016
Accepted 2 June 2016
Available online 9 June 2016

Keywords:
Quantum–classical transition
Wave packet interference
Quantum trajectory
Classical time-dependent Schrödinger equation
Quantum Hamilton–Jacobi equation

ABSTRACT

The quantum–classical transition for wave packet interference is investigated using a hydrodynamic description. A nonlinear quantum–classical transition equation is obtained by introducing a degree of quantumness ranging from zero to one into the classical time-dependent Schrödinger equation. This equation provides a continuous description for the transition process of physical systems from purely quantum to purely classical regimes. In this study, the transition trajectory formalism is developed to provide a hydrodynamic description for the quantum–classical transition. The flow momentum of transition trajectories is defined by the gradient of the action function in the transition wave function and these trajectories follow the main features of the evolving probability density. Then, the transition trajectory formalism is employed to analyze the quantum–classical transition of wave packet interference. For the collision-like wave packet interference where the propagation velocity is faster than the spreading speed of the wave packet, the interference process remains collision-like for all the degree of quantumness. However, the interference features demonstrated by transition trajectories gradually disappear when the degree of quantumness approaches zero. For the diffraction-like wave packet interference, the interference process changes continuously from a diffraction-like to collision-like case when the degree of quantumness gradually decreases. This study provides an insightful trajectory interpretation for the quantum–classical transition of wave packet interference.

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http://dx.doi.org/10.1016/j.aop.2016.06.001
0003-4916/

1. Introduction

Various trajectory approaches have been developed to study quantum dynamical processes because these methods can provide new physical insights into the dynamics. As a trajectory formulation of quantum mechanics [1–3], Bohmian mechanics has been utilized to analyze a diverse range of physical processes through computing and interpreting *real-valued* quantum trajectories from a precomputed wave function, including the dissociation of molecules at metal surfaces, atom diffraction by surfaces, quantum nonlocality, quantum interference, the geometric phase, and the Airy wave packet dynamics [4–14]. On the other hand, the quantum trajectory method (QTM) has been developed as a computational tool to generate the wave function by propagating quantum trajectories through the integration of the hydrodynamic equations *on the fly* [15–17]. In addition, the bipolar representation of the total wave function has been used to reconcile semiclassical and Bohmian mechanics for stationary states and wave packet dynamics [18–26]. Recently, dissipative Bohmian trajectories have been analyzed within the Caldirola-Kanai framework [27]. In addition, the nonlinear Schrödinger–Langevin equation has been generalized for quantum processes in the presence of nonlinear friction and a heat bath [28,29], and this equation has been solved for the ground state of quantum systems by propagating quantum trajectories [30,31]. Remarkable progress has been made in the development and application of real-valued quantum trajectories for providing an analytical, interpretative, and computational framework for quantum dynamical problems [3,32–35].

In contrast with the real-valued QTM, complex-valued quantum trajectories have been developed as both the analytic and synthetic approaches to quantum dynamical problems. Based on the complex quantum Hamilton–Jacobi formalism [36,37], the complex QTM has been used to analyze both stationary bound and scattering state problems [38–52]. Quantum interference demonstrated by the head-on collision of two Gaussian wave packets has been thoroughly analyzed using complex quantum trajectories [53–55]. In computational applications, the complex QTM has been applied to one-dimensional and multi-dimensional wave packet scattering problems [56–68]. In addition, this approach has been used to describe the interference effects and node formation in the wave function [69,70], to calculate energy eigenvalues [71], and to improve the complex time-dependent Wentzel–Kramers–Brillouin (WKB) method [72–74]. Furthermore, the complex QTM has been applied to the dissipative dynamics described by a stochastic Liouville–von Neumann equation with complex noise forces [75] and to nonadiabatic molecular dynamics [76,77].

In Bohmian mechanics, the wave function is first written in terms of the real amplitude and the real action function. Substituting the polar decomposition of the wave function into the time-dependent Schrödinger equation (TDSE) yields a system of two coupled partial differential equations, the continuity equation and the quantum Hamilton–Jacobi equation (QHJE). In contrast with the classical Hamilton–Jacobi equation, the QHJE includes not only the kinetic energy and the classical potential but also the quantum potential. It is the quantum potential that brings all quantum effects into the hydrodynamic formulation.

The classical analog of the TDSE has been derived to provide a field description for classical dynamics [78–82]. The *classical* TDSE is obtained by subtracting a quantum potential term in the TDSE, and this additional term has the effect of erasing quantum effects. Because the additional term is nonlinear, the superposition principle does not hold for the classical TDSE. The classical TDSE can be converted into the classical hydrodynamic equations of motion. Although the dynamics are classical, the *classical* wave function satisfying the classical TDSE leads to an approximate quantum probability amplitude. The classical TDSE for an ensemble of classical trajectories has been thoroughly discussed using a quantum language [3,33].

In a previous study [83], a nonlinear quantum–classical transition equation has been proposed by introducing a *degree of quantumness* ranging from zero to one into the classical TDSE. When the degree of quantumness is equal to one, the transition equation reduces to the TDSE. On the contrary, we recover the classical TDSE when the degree of quantumness completely disappears. Hence, the transition equation provides a continuous description of physical systems for the quantum–classical transition. In addition, it has been shown that the nonlinear quantum–classical transition equation is equivalent to a linear scaled TDSE with a rescaled Planck's constant.