Vol 15 No 5, May 2006
1009-1963/2006/15(05)/0919-04

Chinese Physics

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Semiclassical propagator and van Vleck determinant in a mixed position–momentum space

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(Received 18 September 2005; revised manuscript received 22 November 2005)

In this paper a semiclassical propagator in a mixed position–momentum space is derived in the formalism of Maslov's multi-dimensional semiclassical theory. The corresponding mixed van Vleck determinant is also given explicitly. The propagator can be used to locally fix semiclassical divergences in singular regions of configuration space. It is shown that when a semiclassical propagator is transformed from one representation to another, its form is invariant.

Keywords: semiclassical theory, propagator, mixed space
PACC: 0365S, 3100

It is well known that WKB approximation is a standard semiclassical method and has been successfully used in many physical problems.[1,2] But it is usually confined to one-dimensional cases. There has long been a need for the development of a method that can be used to deal with multi-dimensional problems. In last two decades, the Maslov and Fedoriuk (MF) n-dimensional semiclassical theory[3] has achieved a great progress in this direction and has been used successfully in the atomic and molecular physics.[4−6] Recent applications of semiclassical theory for quantum chaos and Rydberg atoms and/or ions is external fields can be found in Refs.[7–11] MF's theory emphasizes a suitable choice of representation space (usually a mixed position–momentum space) to overcome the semiclassical diversity in configuration or momentum space. Delos has shown how to construct a uniform semiclassical wave function by using MF's approach.[6] The semiclassical propagator in configuration space, known as van Vleck formula, has been acquired by many authors from different starting points.[12−16] But it can not work in the singular regions such as near caustics or foci of classical trajectories. To overcome the difficulty, Keller proposed a complex trajectory formalism.[17] But a complex trajectory has not a definite physical meaning in classical mechanics. In fact, such divergence is not due to semiclassical theory itself, but that configuration space is not suitable Lagrangian coordinate plane of the Lagrange manifold in phase space.[3,6] The divergence can be repaired by transforming the wavefunction or propagator into a momentum or mixed position–momentum space. Maslov and Fedoriuk have shown that a semiclassical wavefunction or propagator is invariant when it is transformed from position representation to momentum or mixed position–momentum representation under stationary phase approximation.[3] Gutzwiller has given a formal transforming formula of propagator to momentum space.[6] For multi-dimensional problems, a mixed position–momentum representation is more suitable and it contains position and momentum representations as two special cases. In this paper we will show how to calculate explicitly a semiclassical propagator in a mixed position–momentum space and then construct a uniform semiclassical propagator which is finite even at any boundaries between classically allowed and forbidden regions where the primitive propagator in configuration space is divergent.

A uniform semiclassical propagator can be constructed by the following steps: firstly, at any singular regions in configuration space, we transform the primitive propagator into a suitably chosen mixed space, then a finite propagator in the mixed space can be constructed; finally we transform it back into configuration space and sew it with the primitive propagator smoothly to construct a uniform semiclassical propagator. The method can be used to construct a uni-

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form semiclassical Green function in the same way.[18] In the following we will explicitly accomplish the construction.

For simplicity's sake we consider a single particle without spin in n-dimensional configuration space, and its Hamiltonian is independent of time. For given energy, the propagator $K(q'', q', t - t_0)$ satisfies the inhomogeneous equation

$$\left[\mathrm{i}\hbar\frac{\partial}{\partial t} - H\right] K(q'', q', t - t_0) = \mathrm{i}\hbar\delta(q'' - q')\delta(t - t_0), \tag{1}$$

where q' and t_0 are the initial position and time, q'' and t are the final position and time. Without loss of generality, take $t_0 = 0$, then $K(q'', q', t - t_0)$ becomes $K(q'', q', t)$. The semiclassical approximation K_c of K is given by Van Vleck formula[16]

$$K_\mathrm{c}(q'', q', t) = \frac{1}{(2\pi\hbar)^{n/2}} \sum_{\text{class.traj.}} (|C_R|)^{1/2} \times \exp\left[\frac{\mathrm{i}}{\hbar}\left(R - \mu\frac{\pi}{2}\right)\right], \tag{2}$$

where

$$R(q'', q', t) = \int_0^t L(q, \dot{q}, t)\mathrm{d}t \tag{3}$$

is the classical action evaluated along the classical path which leads from q' to q'' at the given time t and μ is the Maslov index which is related to the topological properties of the ray of trajectories. Its intrinsic geometrical properties have been discussed in detail by Littlejohn and co-workers.[19,20] The summation in Eq.(2) is over all classical trajectories from q' to q''. The Van Vleck determinant is defined as

$$C_R = \left|-\frac{\partial^2 R}{\partial q' \partial q''}\right|. \tag{4}$$

According to quantum mechanics, a propagator must be finite everywhere. However, the primitive semiclassical propagator of Eq.(2) has singularities at any boundary between classically allowed and forbidden regions and at any caustics or focus of classical trajectories. The reason for such singularity is not due to the semiclassical theory itself, but because the configuration representation is not suitable any more in these regions. When it is transformed into momentum or mixed position–momentum space, such singularities can be fixed. It has been shown that there 'almost always' exists a representation in which the semiclassical approximation does not diverge in these singular regions.[3,6]

We choose mixed coordinates (p_α, q_β), where $\alpha = 1, \cdots, k$ and $\beta = k + 1, \cdots, n$. In other words, they are disjoint sets. So the mixed coordinates contain no canonical conjugate pairs. The propagator in the mixed space can be obtained from the counterpart in configuration space by partial Fourier transformation. The propagator $F(p''_\alpha, q''_\beta, p'_\alpha, q'_\beta)$ from $(p'_\alpha, q'_\beta)$to (p''_α, q''_β) is defined by

$$K(p''_\alpha, q''_\beta, p'_\alpha, q'_\beta, t) = (2\pi\hbar)^{-k} \int \mathrm{d}q''_\alpha \int \mathrm{d}q'_\alpha K(q'', q', t) \times \exp[\mathrm{i}(p'_\alpha q'_a - p''_\alpha q''_\alpha)/\hbar]. \tag{5}$$

Its semiclassical approximation $K_\mathrm{c}(p''_\alpha, q''_\beta, p'_\alpha, q'_\beta, t)$ can be obtained by inserting $K_\mathrm{c}(q'', q')$ into Eq.(5) and evaluating the integral by k-dimensional stationary phase approximation (SPA). Firstly, we calculate the integral on q'_α, that is

$$K_\mathrm{c}(q'', p'_\alpha, q'_\beta, t) \approx (2\pi\hbar)^{-k/2} \int \mathrm{d}q'_\alpha K_\mathrm{c}(q'', q', t)\exp(\mathrm{i}p'_\alpha q'_\alpha/\hbar). \tag{6}$$

Inserting Eq.(2) into the expression, we find that the exponent becomes the product

$$\tilde{R} = R + p'_\alpha q'_\alpha \tag{7}$$

and the factor $\mathrm{i}/\hbar$. It is noted that we use a single symbol to denote the exponent before and after the SPA. For convenience, the Maslov index and summation over classical trajectories have been dropped temporarily. The stationary phase (SP) points $q'_{\alpha 0}$ satisfy

$$\left.\frac{\partial R}{\partial q'_\alpha}\right|_{q'_{\alpha 0}} = -p'_\alpha, alpha = 1, \cdots, k. \tag{8}$$

After SPA the pre-exponential factor can be written as

$$\frac{1}{(2\pi\mathrm{i}\hbar)^{n/2}} \frac{(2\pi\mathrm{i}\hbar)^{k/2}}{(2\pi\hbar)^{k/2}} (C_R)^{1/2} \left(\frac{\partial^2 R}{\partial^2 q'_\alpha}\right)^{-1/2} = \frac{\mathrm{i}^{k/2}}{(2\pi\mathrm{i}\hbar)^{n/2}} (C_R)^{1/2} \left(-\frac{\partial q'_\alpha}{\partial p'_\alpha}\right)^{1/2}. \tag{9}$$

To simplify the expression further, we rewrite C_R as

$$C_R = \begin{vmatrix} \dfrac{\partial^2 R}{\partial q'_\alpha \partial q''_\alpha} & \dfrac{\partial^2 R}{\partial q'_\alpha \partial q''_\beta} \\ \dfrac{\partial^2 R}{\partial q'_\beta \partial q''_\alpha} & \dfrac{\partial^2 R}{\partial q'_\beta \partial q''_\beta} \end{vmatrix} \tag{10}$$

and the second derivatives of R now should be replaced by the derivatives of $\tilde{R}$. To achieve this replacement, we can use the following relations

$$\begin{aligned}\frac{\partial R}{\partial q'_\alpha} &= -p'_\alpha,\\ \frac{\partial \tilde{R}}{\partial q''_\alpha} &= \frac{\partial R}{\partial q''_\alpha},\\ \frac{\partial \tilde{R}}{\partial q''_\beta} &= \frac{\partial R}{\partial q''_\beta}.\end{aligned} \tag{11}$$

Inserting Eqs.(10) and (11) into Eq.(9), we get

$$\begin{aligned}&\frac{(-\mathrm{i})^{k/2}}{(2\pi\mathrm{i}\hbar)^{n/2}}\begin{vmatrix}\dfrac{\partial^2\tilde{R}}{\partial p'_\alpha\partial q''_\alpha} & \dfrac{\partial^2\tilde{R}}{\partial p'_\alpha\partial q''_\beta}\\ \dfrac{\partial^2\tilde{R}}{\partial q'_\beta\partial q''_\alpha} & \dfrac{\partial^2\tilde{R}}{\partial q'_\beta\partial q''_\beta}\end{vmatrix}^{1/2}\\ &\equiv \frac{(-\mathrm{i})^{k/2}}{(2\pi\mathrm{i}\hbar)^{n/2}}(C_{\bar{R}})^{1/2}.\end{aligned} \tag{12}$$

It is noted that all R have been replaced by $\tilde{R}$. After SPA, the integral in Eq.(6) becomes

$$K_{\mathrm{c}}(q'', p'_\alpha, q'_\beta, t) = \frac{(-\mathrm{i})^{k/2}}{(2\pi\mathrm{i}\hbar)^{n/2}}(C_{\bar{R}})^{1/2}\exp\left(\frac{\mathrm{i}}{\hbar}\tilde{R}\right), \tag{13}$$

where

$$\begin{aligned}\tilde{R}(q'', p'_\alpha, p'_\beta, t) =& R(q'', q'_{\alpha 0}(q'', p'_\alpha, q'_\beta, t), q'_\beta, t)\\ &+ p'_\alpha q'_{\alpha 0}(q'', p'_\alpha, q'_\beta, t)\end{aligned} \tag{14}$$

is the value of Eq.(7) at the first SP point. Secondly, we again approximate the integral over q''_α by SPA to obtain the mixed propagator

$$\begin{aligned}&K_{\mathrm{c}}(p''_\alpha, q''_\beta, p'_\alpha, q'_\beta, t)\\ \approx&(2\pi\hbar)^{-k/2}\int \mathrm{d}q''_\alpha K_{\mathrm{c}}(p'', p'_\alpha, q'_\beta, t)\\ &\times\exp(-\mathrm{i}p''_\alpha q''_\alpha/\hbar).\end{aligned} \tag{15}$$

The exponent part of the integrand is

$$\bar{R} = \tilde{R} - p''_\alpha q''_\alpha. \tag{16}$$

The SP points no satisfy

$$\left.\frac{\partial\tilde{R}}{\partial q''_\alpha}\right|_{q''_{\alpha 0}} = p''_\alpha,\ \alpha = 1, \cdots, k. \tag{17}$$

The relations in Eq.(11) are replaced by

$$\begin{aligned}\frac{\partial\bar{R}}{\partial q''_\alpha} &= p''_\alpha,\\ \frac{\partial\bar{R}}{\partial p'_\alpha} &= \frac{\partial\tilde{R}}{\partial p'_\alpha},\\ \frac{\partial\bar{R}}{\partial q'_\beta} &= \frac{\partial\tilde{R}}{\partial q'_\beta},\end{aligned} \tag{18}$$

which leads to replacement of the derivatives with respect to q''_α in the first column of $C_{\bar{R}}$ by the ones to p''_α and the replacement of all $\tilde{R}$ by $\bar{R}$. The pre-exponential factor then becomes

$$\begin{aligned}&\frac{1}{(2\pi\mathrm{i}\hbar)^{n/2}}\begin{vmatrix}\dfrac{\partial^2\bar{R}}{\partial p'_\alpha\partial p''_\alpha} & \dfrac{\partial^2\bar{R}}{\partial p'_\alpha\partial q''_\beta}\\ \dfrac{\partial^2\bar{R}}{\partial q'_\beta\partial p''_\alpha} & \dfrac{\partial^2\bar{R}}{\partial q'_\beta\partial q''_\beta}\end{vmatrix}^{1/2}\\ &\equiv \frac{1}{(2\pi\mathrm{i}\hbar)^{n/2}}(C_{\bar{R}})^{1/2}.\end{aligned} \tag{19}$$

It is noted the factor in Eq.(12) has been cancelled by the second SPA integration. We have to emphasize that $C_{\bar{R}}$ is just the van Vleck determinant in the position–momentum space. Therefore, the final propagator in the mixed space is

$$\begin{aligned}K_{\mathrm{c}}(p''_\alpha, q''_\beta, p'_\alpha, q'_\beta, t) =& \frac{1}{(2\pi\hbar)^{n/2}}\sum_{\text{class.traj.}}(|C_{\bar{R}}|)^{1/2}\\ &\times\exp\left[\frac{\mathrm{i}}{\hbar}\left(\bar{R} - \bar{\mu}\frac{\pi}{2}\right)\right],\end{aligned} \tag{20}$$

where

$$\begin{aligned}\bar{R}(p''_\alpha, q''_\beta, p'_\alpha, q'_\beta, t) =& \tilde{R}(q''_\alpha(p''_\alpha, q''_\beta, p'_\alpha, q'_\beta, t), q''_\beta, p'_\alpha, q'_\beta, t) - p''_\alpha q''_\alpha(p''_\alpha, q''_\beta, p'_\alpha, q'_\beta, t)\\ =& R(q''_\alpha(p''_\alpha, q''_\beta, p'_\alpha, q'_\beta, t), q''_\beta, q'_\alpha(p''_\alpha, q''_\beta, p'_\alpha, q'_\beta, t), q'_\beta, t)\\ &+ p'_\alpha q'_\alpha(p''_\alpha, q''_\beta, p'_\alpha, q'_\beta, t) - p''_\alpha q''_\alpha(p''_\alpha, q''_\beta, p'_\alpha, q'_\beta, t)\end{aligned}$$

is the value of Eq.(7) at the second SP point where we used the same symbol. Its concise form is

$$\bar{R} = R + p'_\alpha q'_\alpha - p''_\alpha q''_\alpha. \tag{21}$$

In Eq.(20) the Maslov index $\bar{\mu}$ has been added and it related the topological properties of classical trajectories in the mixed space. The summation over classical trajectories has also been added. Comparing Eq.(20) with Eqs.(2) and (22), we can find that each semiclassical propagator consists of an amplitude matrix and an exponential function on corresponding classical action respectively. We conclude that the semiclassical function is invariant in form when it is transformed from one representation to another.

Formula (20) is a unified expression. If $\alpha = 0$, $\beta = 1, \cdots, n$, it will recover to Eq.(2), the propagator in configuration space. On the other hand, if $\alpha = 1, \cdots, n, \beta = 0$, we have the propagator in momentum space

$$K_{\mathrm{Fc}}(p'', p', t) = \frac{1}{(2\pi\hbar)^{n/2}} \sum_{\text{class.traj.}} (|C_T|)^{1/2} \times \exp\left[\frac{\mathrm{i}}{\hbar}\left(T - \nu\frac{\pi}{2}\right)\right], \qquad (22)$$

where

$$T(p'', p', t) = R(q'', q', t) - p'q' - p''q'' \qquad (23)$$

is the classical action along the classical path from p' to p'' at the given time t, and ν is the Maslov index calculated in momentum space. Usually, $\nu \neq \mu$ because of the different topological properties of trajectories between configuration and momentum spaces. The determinant is defined in an analogous way as

$$C_T = \left| -\frac{\partial^2 T}{\partial p' \partial p''} \right|. \qquad (24)$$

Equation (23) is just the Gutzwiller's semiclassical propagator in momentum space.[4]

For most semiclassical physical problems, it is convenient to work in configuration space. Equation (2) usually works quite well in most regions. But in some regions, such as near caustics and foci of classical trajectories, it will be divergent. In these regions, we can 'almost always'[3,6] choose a suitable set of mixed position–momentum coordinates to construct a mixed propagator which is finite. From this function, an accurate configuration space propagator can be constructed by an inverse partial Fourier transformation,

$$K_{\mathrm{c}}(q'', q', t) = (2\pi\hbar)^{-k} \int \mathrm{d}p''_\alpha \int \mathrm{d}p'_\alpha K_{\mathrm{c}}(p''_\alpha, q''_\beta, p'_\alpha, q'_\beta, t) \times \exp[\mathrm{i}(-p'_\alpha q'_a + p''_\alpha q''_\alpha)/\hbar]. \qquad (25)$$

Then we can sew it with the primitive propagator smoothly to get a uniform propagator.

The semiclassical propagator in mixed position–momentum spaces have been successfully used to calculate the ring structure of electron flux of photodetachment microscope.[21]

In summary, we have obtained a semiclassical propagator in a mixed position–momentum space explicitly and it can be used to locally fix semiclassical divergences in singular regions of configuration space. The explicit expression is quite useful in the study of quantum chaos, atomic and molecular physics and chemical physics.

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