International Journal of Engineering, Mathematical and Physical Sciences
ISSN: 2517-9934
Vol:5, No:11, 2011

One scheme of Transition Probability Evaluation

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***Abstract*—**In present work are considered the scheme of evaluation the transition probability in quantum system. It is based on path integral representation of transition probability amplitude and its evaluation by means of a saddle point method, applied to the part of integration variables. The whole integration process is reduced to initial value problem solutions of Hamilton equations with a random initial phase point. The scheme is related to the semiclassical initial value representation approaches using great number of trajectories. In contrast to them from total set of generated phase paths only one path for each initial coordinate value is selected in Monte Karlo process.

***Keywords*—**Path integral, saddle point method, semiclassical approximation, transition probability

I. Introduction

SEMICLASSICAL approximations are widely used in the quantum physicist. There is a huge number of works devoted to theory and applications of this method. There are many approaches to its justification. The popular approach is based on path integral evaluation by means of the stationary phase or the saddle point methods [1]-[10]. A variety of forms of path integral leads to various semiclassical approximations.

One of the problems discussed often in context of semiclassical approximation is the search of the stationary paths. It is known that search schemes based on initial value representation (IVR) has many advantages in comparison with ones based on boundary value representation (BVR). The popular IVR approaches using wave packets are Herman-Kluk (HK) and Eric Heller (EH) methods [11]-[17]. In connection with HK approximation in [16] it was compared methods using single and a great number of trajectories. The last ones gives better results for wider rang of the physical problem parameters.

In the present work we consider the scheme of the transition probability evaluation. It is based on path integral representation of transition probability and its evaluation by means of the saddle point method, applied to the part of integration variables. The scheme is related to the semiclassical IVR approaches using great number of trajectories.

II. Method Description

The various forms of path integral and corresponding semiclassical approximations are based on the concept of operator's symbols. In atomic physics *qp*-, *pq*- and Weyl (symmetric) symbols and symbols associated with generalized coherent states are usually treated [18]-[24].

Our scheme is independent of the particular symbols choice. For definiteness we use *qp*-symbols. This system has some advantage because usually the Hamiltonian has the form of operator given in *qp*-normal form for which the symbol calculation is trivial. The calculation of the other symbols of such operators can be rather difficult. For example, in case of widely used canonical group coherent states (in other terms coherent states of harmonic oscillators or Gaussian wave packets) calculation of symbols needs Fock-Bargmann integral transform.

The transition probability amplitude between initial $\psi_i(t')$ and final $\psi_f(t)$ states has following form of path integral in phase space

$$A_{if} = \int \psi_f^*(q_t,t)\exp\left(\frac{i}{\hbar}S(q.p)\right)\psi_i(q_{t'},t')\,dqdp \qquad (1)$$

with Hamilton action

$$S = \int (pdq - Hdt).$$

We use finite-dimensional approximations of path integral. Problems of their convergence were considered in a number of works, for example in [21]. Finite-dimensional approximation of the transition probability amplitude looks like (1) with an integration over discrete phase trajectories

$$q = (q_0, \dots, q_{l+1}), \quad p = (p_0, \dots, p_l),$$
$$dqdp = dq_{l+1}\bigwedge_{j=0}^{l}\frac{dq_j dp_j}{(2\pi i\hbar)^n}, \qquad (2)$$

where n is the dimension of coordinate space and

$$q_0 = q_{t'}, \quad q_{l+1} = q_t,$$
$$S = \sum_{j=0}^{l} p_j \Delta q_j - \sum_{j=0}^{l-1} H(q_{j+1}, p_j, t_j)\Delta t,$$
$$\Delta t = \frac{t-t'}{l}, \quad \Delta q_j = q_{j+1} - q_j$$

is the integral sum for the Hamilton action with Hamiltonian *H*.

In case of Hamiltonian with quadratic kinetic term integration over momentum in path integral (1) can be done analytically and leads to path integral in configuration space. At that

$$dq = dq_{l+1}\bigwedge_{j=0}^{l}\gamma^{-n/2}dq_j,$$

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$$\gamma = 2\pi i\,\varepsilon, \qquad \varepsilon = \frac{\Delta t\ \hbar}{m},$$

$$S = \sum_{j=0}^{l-1} \Delta t \left(\frac{m}{2}\left(\frac{\Delta q_j}{\Delta t}\right)^2 - V\left(q_{j+1}, t_j\right) \right)$$

is the integral sum for Lagrange action with interaction potential V.

The complexity of numerical estimation of Feynman type path integral is caused besides dimensionality by oscillating character of the integrand containing a complex exponential. For example this leads to difficulties in Monte Karlo integration, which is widely used for Wiener path integrals with real exponential. For this reason there are few works using this approach for Feynman path integrals [25]. More commonly is used estimation by means of the stationary phase or the saddle point methods.

Firstly these methods can be applied to whole path integral (all integration variables). Such approach was used in some works, for example [3], [26]. It gives reliable results when there exist small number of separate essential saddle point (or stationary) paths, i.e. when saddle points are not degenerate.

Another possibility is to apply the stationary phase or the saddle point methods to part of integration variables only with direct integration over the rest ones. In this case the part of trajectory is stationary and the remained part is virtual. The probability of saddle point paths degeneracy is lower for lower number of variables. We consider this approach in this paper.

Generally the choice of separation into stationary and virtual parts of trajectory can be arbitrary, but let us note, that one of coordinates is detached in path differential (2). This suggests to perform direct integration in (1) over one of coordinates and to apply the saddle point method to the rest part of integration variables. It is convenient to take initial coordinate – q_0 as virtual.

For application of the saddle point method it is useful to extract fast varying exponential part in initial wave function

$$\psi_f^*(q) = P_f(q)\exp\left(\frac{i}{\hbar} S_f(q)\right)$$

and to rewrite (1) in the form

$$A_{if} = \int_D P_f\left(q_{l+1}\right)\exp\left(\frac{i}{\hbar}\Theta(q,p)\right)\psi_i(q_0)\,dqdp \qquad (3)$$

with phase function

$$\Theta(q,p) = S_f\left(q_{l+1}\right) + S(q,p). \qquad (4)$$

Let's notice, that in general the phase of wave function can be complex and hence the stationary phase method can be inapplicable and the saddle point method is to be applied naturally.

The problems of the saddle point method are well known and are considered, in particular, in [2]. It is assumed an analytic continuation of an integrand so that an integration domain $D = \{q, p \mid \mathrm{Im}(q,p) = 0\}$ could be included in analyticity domain and could be deformed to include the saddle points giving the dominant contribution to an integral. Generally the integrand either doesn't have analytic continuation or the domain of analyticity doesn't contain the primary integration domain and hence the path integral on a deformed domain and the primary path integral are different ones. Another problem is the existence of the suitable deformed integration domain containing the significant saddle points. This topological part is most difficult and crucial in the saddle point method [27]. The partial solution of these problems is to use approximations with entire functions [2]. Further we suppose that an integrant has required analytic properties.

The saddle point integration of (3) leads to the following expression of the transition probability amplitude in form of integral over initial coordinate q_0

$$A_{if} \approx \int P_f\left(q_{l+1}\right)\left(\det\left(\Theta 2(q,p)\right)\right)^{-1/2}\exp\left(\frac{i}{\hbar}\Theta(q,p)\right)\psi_i(q_0)\,dq_0 \qquad (5)$$

with integrand taken on a saddle point path

$$q' = \left(q_1, \ldots, q_{l+1}\right),\ p' = \left(p_0, \ldots, p_l\right),$$

being a solution of the stationary phase equation with given initial coordinate q_0

$$\Theta 1 = \frac{\partial\Theta(q,p)}{\partial(q',p')} = 0, \qquad (6)$$

$$\Theta 2 = \frac{\partial^2\Theta(q,p)}{\partial(q',p')^2}. \qquad (7)$$

It is supposed that the second variation matrix (7) of the phase function (4) is nondegenerate and that the solution of the stationary phase equation (6) with given initial coordinate q_0 is unique.

The choice of a root branch in (5) and its connection with path index is considered in [2]. Precisely the prefactor with determinant can be written in following form. Let us designate the eigenvalues of the second variation matrix $\Theta 2$ as

$$\mu = |\mu|\exp\left(i\cdot\arg(\mu)\right), \quad (-\pi < \arg \le \pi),$$

then the prefector can be represented as

$$\left(\det(\Theta 2)\right)^{-1/2} = \left|\det(\Theta 2)\right|^{-1/2}\exp\left(-\frac{\pi i}{2} Ind\right),$$

where

$$Ind = \frac{1}{\pi}\sum_{\mu}\arg(\mu).$$

Generally the last value is real, but for the pure real matrix $\Theta 2$ it is integer and $Ind = ind\ (\mathrm{mod}\ 4)$, where ind – is Maslov's index of the path.

The stationary phase equation (6) with given initial coordinate can be represented in the form of a boundary value problem for finite-difference set of Hamilton equations in a complex phase space

$$\frac{\Delta q_j}{\Delta t} = \frac{\partial H(q_{j+1}, p_j)}{\partial p_j}$$
$$\frac{\Delta p_j}{\Delta t} = -\frac{\partial H(q_{j+1}, p_j)}{\partial q_{j+1}}$$
$$j = 0, \dots l-1$$

with boundary conditions including given initial coordinate q_0 and a final condition

$$p_l = \frac{\partial S_f}{\partial q_{l+1}}. \quad (8)$$

This BVR problem can be solved by means of the multiple shooting method, which efficiently converts it to IVR problem. For this purpose the set of Hamilton equations with initial phase points (q_0, p_0) is solved and the residual for a final condition (8) is minimized at variation of initial momentum (complex generally) p_0 at each given initial coordinate q_0. It can be done on the basis of a random sampling of initial momentum.

This sampling can be superposed with Monte Karlo integration over initial coordinate in (5). Thus a whole process is reduced to IVR problem solutions of Hamilton equations with a random initial phase point (q_0, p_0). From total set of generated phase paths in expression (5) are selected only one path for each initial coordinate q_0 value.

The prefactor with determinant in (5) can be found on base of the procedure similar to those described in [2].

III. Conclusion

Presented above calculation scheme uses the separation of path integral integration variables to those integrated by the saddle point method (in particular all variables excluding initial coordinate) and the directly integrated rest ones (in particular initial coordinate). The whole process is represented in form of IVR problem solutions of Hamilton equations with a random initial phase point (q_0, p_0).

Generally the choice of separation into stationary and virtual parts of trajectory can be arbitrary. For example one can make direct integration over initial and final coordinates. It is worthy to note that conversion of the last scheme to IVR form leads to approximation, which is close to very popular HK and related ones.

However it is difficult to make better numerical evaluation of integrals with oscillating integrand than gives the stationary phase or the saddle point methods. So in case of oscillating final wave function (frequent case) direct integration over final coordinate may be inexpedient and it is better to include it into saddle point integration.

Apparently there exist optimal separation for each type of integrand.

Considered approach is related to efficient IVR semiclassical methods, such as HK and EH and some other approaches using wave packets [1]-[10]. But unlike the major part of mentioned methods complex phase paths are used. Besides from total set of generated phase paths only one path for each initial coordinate q_0 value is selected in expression (5).

We tested this scheme in calculation of photo-ionization probability in Hydrogen atom. Preliminary results shows that approach gives better results for wider rang of photo-pulse parameters than the scheme with the saddle point integration of (3) over all variables and few saddle point paths [26].

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