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THE SEMICLASSICAL APPROXIMATION OF MULTIPLE FUNCTIONAL INTEGRALS

Abstract. In this paper, we study the semiclassical approximation of multiple functional integrals. The integrals are defined through the Lagrangian and the action. Of all possible trajectories, the greatest contribution to the integral is given by the classical trajectory $\vec{x}_{cl}$ for which the action S takes an extremal value. The classical trajectory is found as a solution of the multidimensional Euler – Lagrange equation. To calculate the functional integrals, the expansion of the action with respect to the classical trajectory is used, which can be interpreted as an expansion in powers of Planck's constant. The numerical results for the semiclassical approximation of double functional integrals are given.

Keywords: multiple functional integrals, semiclassical approximation, action, classical trajectory

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КВАЗИКЛАССИЧЕСКАЯ АППРОКСИМАЦИЯ КРАТНЫХ ФУНКЦИОНАЛЬНЫХ ИНТЕГРАЛОВ

Аннотация. Исследуется квазиклассическая аппроксимация кратных функциональных интегралов. Интегралы определяются через лагранжиан и действие. Из всех возможных траекторий наибольший вклад в интеграл дает классическая траектория $\vec{x}_{cl}$, для которой действие S принимает экстремальное значение. Классическая траектория находится как решение многомерного уравнения Эйлера – Лагранжа. Для вычисления функциональных интегралов используется разложение действия относительно классической траектории, которое может интерпретироваться как разложение по степеням постоянной Планка. Приводятся численные результаты для квазиклассической аппроксимации двукратных функциональных интегралов.

Ключевые слова: кратные функциональные интегралы, квазиклассическая аппроксимация, действие, классическая траектория

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Introduction. Ever since Feynman in 1942 introduced path integration methods to physics, functional integration has become a common tool in physics as well as in some branches of mathematics. We do not write a review about functional integrals. We note the wide application of functional integrals in quantum mechanics and field theory [1–3], in the theory of stochastic differential equations [4–6], and in many other areas [7]. Methods for the approximate calculation of functional integrals were considered in [8, 9].

The semiclassical approximation (or the Wentzel – Kramers – Brillouin (WKB) approximation) is used in quantum mechanics to approximate the solution of the one-dimensional time-independent Schrödinger equation by expanding it in a series of powers of Planck's constant $\hbar$. The semiclassical approximation of functional integrals with respect to the conditional Wiener measure was considered in [10, 11]. In this paper, we study the semiclassical approximation of multiple functional integrals. The integrals are defined in terms of the Lagrangian and the action. The semiclassical approximation uses an expansion of the action with respect to the classical trajectory, which can be interpreted as an expansion in powers of Planck's constant. In the case of multiple functional integrals, the classical trajectory is found as a solution to the multidimensional Euler – Lagrange equation. We consider the semiclassical approximation using the example of double functional integrals. If necessary, the method can be generalized to integrals of higher multiplicity.

Analytical results. For the functional integral, we will use the notation

$$K(\vec{x}_s,\vec{x}_t)=\int \exp\left\{-\frac{1}{\hbar}S\right\}D[\vec{x}], \tag{1}$$

where $S=\int_s^t L(\dot{\vec{x}},\vec{x},\tau)d\tau$ is an action, $L(\dot{\vec{x}},\vec{x},\tau)$ is a Lagrangian, $\hbar$ is a parameter taking positive real values.

Functional integral (1) can be understood as a limit, namely, the integral of the second multiplicity is defined by the equality

$$K(\vec{x}_s,\vec{x}_t)=\lim_{n\to\infty}\int_R (2n-2)\int_R \exp\left\{-\frac{1}{\hbar}\sum_{j=1}^{n}(t_j-t_{j-1})L\left(\frac{x_{1j}-x_{1j-1}}{t_j-t_{j-1}},\frac{x_{2j}-x_{2j-1}}{t_j-t_{j-1}},x_{1j},x_{2j},t_j\right)\right\}\times$$
$$\times\frac{1}{2\pi\hbar(t_n-t_{n-1})}\prod_{j=1}^{n-1}\frac{dx_{1j}dx_{2j}}{2\pi\hbar(t_j-t_{j-1})},$$

where $s=t_0<t_1<\ldots<t_n=t,\ x_{1j}=x_1(t_j),\ x_{2j}=x_2(t_j),\ x_{10}=x_{1s}=x_1(s),\ x_{20}=x_{2s}=x_2(s),\ x_{1n}=x_{1t}=$ $=x_1(t),\ x_{2n}=x_{2t}=x_2(t),\ \vec{x}_s=(x_{1s},x_{2s}),\ \vec{x}_t=(x_{1t},x_{2t})$.

The integral can be interpreted as summation over all trajectories connecting the start and end points. Using the principle of least action [1] to calculate the functional integral, it is possible to select a classical trajectory $\vec{x}_{cl}$ from all possible trajectories for which the action S takes an extreme value. The classical trajectory gives the greatest contribution to the sum. The classical trajectory is found as a solution to the Euler – Lagrange equations

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}_k}\right)-\frac{\partial L}{\partial x_k}=0,\qquad 1\le k\le 2. \tag{2}$$

The semiclassical approximation of functional integrals uses the expansion of the action S with respect to the classical trajectory $\vec{x}_{cl}$:

$$S[\vec{x}(\tau)]\approx S[\vec{x}_{cl}(\tau)]+\frac{1}{2}\delta^2 S[\vec{x}_{cl}(\tau)]. \tag{3}$$

To explain why approximate equality (3) is used, we consider the expansion of the action in the one-dimensional case

$$S[x(\tau)]\approx S[x_{cl}(\tau)]+\frac{1}{2}\frac{\delta^2 S[x_{cl}(\tau)]}{\delta x^2}y^2+\frac{1}{3!}\frac{\delta^3 S[x_{cl}(\tau)]}{\delta x^3}y^3+\ldots,$$

where $y=\delta x,\ x=x_{cl}+\delta x$.

After the introduction of variables $y=\sqrt{\hbar}z$ we get

$$\frac{1}{\hbar}S[x(\tau)]\approx\frac{1}{\hbar}S[x_{cl}(\tau)]+\frac{1}{2}\frac{\delta^2 S[x_{cl}(\tau)]}{\delta x^2}z^2+\sqrt{\hbar}O(z^3).$$

For a small $\hbar$ in the expansion of the action, only terms with zero and second degrees in z can be left, since they contain $\hbar^{-1}$ and $\hbar^0$, and the term with $O(z^3)$ contains $\hbar^{\frac{1}{2}}$.

In the two-dimensional case, the second-order variation $\delta^2 S[\vec{x}_{cl}(\tau)]$ can be written in the following form

$$\delta^2 S[\vec{x}_{cl}(\tau)]=\int_s^t\sum_{i,j=1}^{2}\delta x_i\Lambda_{ij}\delta x_j d\tau,$$

where $\vec{x}=\vec{x}_{cl}+\delta\vec{x}$,

$$\Lambda_{ij}=\left(\frac{\partial^2 L}{\partial x_i\partial x_j}\right)_{\vec{x}_{cl}}+\left(\frac{\partial^2 L}{\partial x_i\partial \dot{x}_j}\right)_{\vec{x}_{cl}}\frac{d}{dt}-\frac{d}{dt}\left(\frac{\partial^2 L}{\partial \dot{x}_i\partial x_j}\right)_{\vec{x}_{cl}}-\frac{d}{dt}\left(\frac{\partial^2 L}{\partial \dot{x}_i\partial \dot{x}_j}\right)_{\vec{x}_{cl}}\frac{d}{dt}.$$

After these transformations, integral (1) can be written as

$$K(\vec{x}_s,\vec{x}_t)=\exp\left\{-\frac{1}{\hbar}S[\vec{x}_{cl}(\tau)]\right\}\int\exp\left\{-\frac{1}{2\hbar}\int_s^t\sum_{i,j=1}^{2}\delta y_i\Lambda_{ij}\delta y_j d\tau\right\}D[\vec{y}], \tag{4}$$

where integration is performed along trajectories $\vec{y}=\delta\vec{x}$ satisfying the conditions $\vec{y}(s)=0, \vec{y}(t)=0$.

The integral in equality (4) can be calculated by analogy with the one-dimensional case [10, 11]:

$$\int\exp\left\{-\frac{1}{2\hbar}\int_s^t\sum_{i,j=1}^{2}\delta y_i\Lambda_{ij}\delta y_j d\tau\right\}D[\vec{y}]=\int\exp\left\{-\frac{1}{2\hbar}\int_s^t\vec{y}\Lambda_{\text{free}}\vec{y}d\tau\right\}D[\vec{y}]\prod_{j=1}^{\infty}\frac{\lambda_{\text{free},j}^{\frac{1}{2}}}{\lambda_j^{\frac{1}{2}}}=\frac{1}{2\pi\hbar(t-t_0)}\prod_{j=1}^{\infty}\frac{\lambda_{\text{free},j}^{\frac{1}{2}}}{\lambda_j^{\frac{1}{2}}},$$

where $\lambda_{\text{free},j}$ are the eigenvalues of the operator

$$\Lambda_{\text{free}}=-\begin{pmatrix}\frac{d^2}{dt^2} & 0\\ 0 & \frac{d^2}{dt^2}\end{pmatrix},$$

λ_j are the eigenvalues of the operator

$$\Lambda=\begin{pmatrix}\Lambda_{11} & \Lambda_{12}\\ \Lambda_{21} & \Lambda_{22}\end{pmatrix}.$$

Thus

$$K(\vec{x}_s,\vec{x}_t)=\exp\left\{-\frac{1}{\hbar}S[\vec{x}_{cl}(\tau)]\right\}\frac{1}{2\pi\hbar(t-t_0)}\prod_{j=1}^{\infty}\frac{\lambda_{\text{free},j}^{\frac{1}{2}}}{\lambda_j^{\frac{1}{2}}}. \tag{5}$$

Numerical results. As an example, we consider the approximate calculation of the functional integral in the case when the Lagrangian has the following form

$$L(\vec{x},\vec{x},\tau)=\frac{1}{2}\left(\dot{x}_1+x_1+a\sin\left(b(x_1+x_2)\right)\right)^2+\frac{1}{2}\left(\dot{x}_2+x_2+a\sin\left(b(x_1+x_2)\right)\right)^2. \tag{6}$$

Let us use the formulas

$$\int_s^t x_j dx_j=\frac{x_j^2(t)-x_j^2(s)}{2}-\hbar\frac{t-s}{2},\quad j=1,2,$$

$$a\int_s^t\sin\left(b(x_1+x_2)\right)dx_1+a\int_s^t\sin\left(b(x_1+x_2)\right)dx_2=$$

$$=-\frac{a}{b}\left[\cos\left(b\left(x_1(t)+x_2(t)\right)\right)-\cos\left(b\left(x_1(s)+x_2(s)\right)\right)\right]-ab\hbar\int_s^t\cos\left(b(x_1+x_2)\right)d\tau.$$

Then the action S can be written as

$$S=\frac{x^2(t)-x^2(s)}{2}-\hbar\frac{t-s}{2}-\frac{a}{b}\left[\cos\left(b\left(x_1(t)+x_2(t)\right)\right)-\cos\left(b\left(x_1(s)+x_2(s)\right)\right)\right]+\overline{S},$$

where

$$\overline{S}=\frac{1}{2}\int_s^t\left[\dot{x}_1^2+\left(x_1+a\sin\left(b(x_1+x_2)\right)\right)^2\right]+\frac{1}{2}\left[\dot{x}_2^2+\left(x_2+a\sin\left(b(x_1+x_2)\right)\right)^2\right]d\tau-ab\hbar\int_s^t\cos\left(b(x_1+x_2)\right)d\tau,$$

the integral in (1) can be written in the following form

$$K(\vec{x}_s,\vec{x}_t)=\int\exp\left\{-\frac{1}{\hbar}S\right\}D[\vec{x}]=$$

$$=\exp\left\{-\frac{x^2(t)-x^2(s)}{2\hbar}+\frac{t-s}{2}+\frac{a}{\hbar b}\Big[\cos\big(b\big(x_1(t)+x_2(t)\big)\big)-\cos\big(b\big(x_1(s)+x_2(s)\big)\big)\Big]\right\}\int\exp\left\{-\frac{\overline{S}}{\hbar}\right\}D[\vec{x}]. \quad (7)$$

Given $\vec{x}_s=\big(x_1(s),x_2(s)\big)=(x_{1s},x_{2s})$, $\vec{x}_t=\big(x_1(t),x_2(t)\big)=(x_{1t},x_{2t})$ the values of the expressions $\frac{x^2(t)-x^2(s)}{2\hbar},-\frac{a}{\hbar b}\Big[\cos\big(b\big(x_1(t)+x_2(t)\big)\big)-\cos\big(b\big(x_1(s)+x_2(s)\big)\big)\Big]$ are known. Therefore, in expression (7) it remains to calculate only the integral $\int\exp\left\{-\frac{\overline{S}}{\hbar}\right\}D[\vec{x}]$ by formula (5) for the action $\overline{S}$.

For the action $\overline{S}$ the Euler – Lagrange equations have the following form

$$\ddot{x}_1-\big[x_1+a\sin\big(b(x_1+x_2)\big)\big]\big[1+ab\cos\big(b(x_1+x_2)\big)\big]-$$

$$-\big[x_2+a\sin\big(b(x_1+x_2)\big)\big]ab\cos\big(b(x_1+x_2)\big)-ab^2\hbar\sin\big(b(x_1+x_2)\big)=0,$$

$$\ddot{x}_2-\big[x_2+a\sin\big(b(x_1+x_2)\big)\big]\big[1+ab\cos\big(b(x_1+x_2)\big)\big]-$$

$$-\big[x_1+a\sin\big(b(x_1+x_2)\big)\big]ab\cos\big(b(x_1+x_2)\big)-ab^2\hbar\sin\big(b(x_1+x_2)\big)=0.$$

The approximate values of the functions $x_{1cl}(\tau)$ and $x_{2cl}(\tau)$, $s\le\tau\le t$, are found by solving these equations using the grid method for solving nonlinear boundary value problems [12].

For the specified Lagrangian Λ_{ij} we have the following form

$$\Lambda_{11}=\Lambda_{22}=V(x_{1cl},x_{2cl})-\frac{d^2}{dt^2},\qquad \Lambda_{12}=\Lambda_{21}=W(x_{1cl},x_{2cl}),$$

where

$$V(x_1,x_2)=\big[1+ab\cos\big(b(x_1+x_2)\big)\big]^2+a^2b^2\cos\big(b(x_1+x_2)\big)^2+$$

$$+ab^2\sin\big(b(x_1+x_2)\big)\big[-x_1-x_2-2a\sin\big(b(x_1+x_2)\big)\big]+ab^3\hbar\cos\big(b(x_1+x_2)\big),$$

$$W(x_1,x_2)=ab\cos\big(b(x_1+x_2)\big)\big[2+2ab\cos\big(b(x_1+x_2)\big)\big]+$$

$$+ab^2\sin\big(b(x_1+x_2)\big)\big[-x_1-x_2-2a\sin\big(b(x_1+x_2)\big)\big]+ab^3\hbar\cos\big(b(x_1+x_2)\big).$$

Note that $V(x_1,x_2)=1+W(x_1,x_2)$.

The operator

$$\Lambda_{\text{free}}=-\begin{pmatrix}\frac{d^2}{dt^2} & 0\\ 0 & \frac{d^2}{dt^2}\end{pmatrix}$$

is approximated by the matrix $\overline{\Lambda}_{\text{free}}=\begin{pmatrix}\overline{\Lambda}_{11\text{free}} & 0\\ 0 & \overline{\Lambda}_{22\text{free}}\end{pmatrix}$, where

$$\overline{\Lambda}_{11\text{free}}=\overline{\Lambda}_{22\text{free}}=h^{-2}\begin{pmatrix}2 & -1 & 0 & \dots & 0\\ -1 & 2 & -1 & \dots & 0\\ \vdots & \vdots & \ddots & \vdots & \vdots\\ 0 & \dots & -1 & 2 & -1\\ 0 & \dots & 0 & -1 & 2\end{pmatrix}$$

are matrices of dimension $(N-1)\times(N-1)$, obtained from the approximation of the second derivative in the node t_j by the expression $h^{-2}(t_{j+1}-2t_j+t_{j-1})$, $h=\frac{t-s}{N}$.

The operators Λ_{ij} are approximated by the matrices $\overline{\Lambda}_{ij}$ of dimension $(N-1)\times(N-1)$, where $\overline{\Lambda}_{11}=\overline{\Lambda}_{22}=\overline{\Lambda}_{11\text{free}}+V$, V is a diagonal matrix of dimension $(N-1)\times(N-1)$ with elements $V_j=V\left(x_{1cl}(jh),x_{2cl}(jh)\right)$, $1\le j\le N-1$ on the diagonal. Also $\overline{\Lambda}_{12}=\overline{\Lambda}_{21}=W$, where W is a diagonal matrix of dimension $(N-1)\times(N-1)$ with elements $W_j=W\left(x_{1cl}(jh),x_{2cl}(jh)\right)$, $1\le j\le N-1$ on the diagonal.

To calculate $\prod_{j=1}^{\infty}\frac{\lambda_{\text{free},j}^{\frac{1}{2}}}{\lambda_j^{\frac{1}{2}}}$ in expression (5), we can use the following equalities

$$\prod_{j=1}^{\infty}\lambda_{\text{free},j}\approx\prod_{j=1}^{N-1}\lambda_{\text{free},j}=(\det\overline{\Lambda}_{11\text{free}})^2,$$

$$\prod_{j=1}^{\infty}\lambda_j\approx\prod_{j=1}^{N-1}\lambda_j=\det\overline{\Lambda}=\det(\overline{\Lambda}_{11}-\det\overline{\Lambda}_{12})\det(\overline{\Lambda}_{11}+\overline{\Lambda}_{12}),$$

where $\overline{\Lambda}_{11}-\overline{\Lambda}_{12}=E+\overline{\Lambda}_{11\text{free}}$, $\overline{\Lambda}_{11}+\overline{\Lambda}_{12}=E+\overline{\Lambda}_{11\text{free}}+2\overline{\Lambda}_{12}$, E is a unit matrix.

Thus, the expression $\prod_{j=1}^{\infty}\frac{\lambda_{\text{free},j}^{\frac{1}{2}}}{\lambda_j^{\frac{1}{2}}}$ is calculated, and by solving the Euler – Lagrange equations for the action $\overline{S}$, the values of the functions $x_{1cl}(\tau)$ and $x_{2cl}(\tau)$, $s\le\tau\le t$ are calculated. The approximate value of the functional integral $K(\vec{x}_s,\vec{x}_t)$ is obtained from formulas (5) and (7).

The application of the semiclassical approximation is illustrated by the following integral with the Lagrangian given by equality (6) and $K(\vec{x}_s,\vec{x}_t)$ is defined by equality (1):

$$E=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}(x_{1t}-x_{2t})K(\vec{x}_s,\vec{x}_t)dx_{1t}dx_{2t}.$$

For $s=0$, $0.5<t\le 2$, $\vec{x}_s=\left(x_1(s),x_2(s)\right)=(1.0)$, $a=0.5$, $b=0.1$, $\hbar=1$ Fig. 1 shows the approximate and exact values of E.

For $s=0$, $0.5<t\le 2$, $\vec{x}_s=\left(x_1(s),x_2(s)\right)=(1.0)$, $a=0.5$, $b=0.1$, $\hbar=0.1$ Fig. 2 shows the approximate and exact values of E.

The exact value of this integral is known, since this integral is equal to the mathematical expectation $E(x_1-x_2)$, where x_1, x_2 is the solution to the system of stochastic differential equations

$$dx_1=\left(-x_1-a\sin\left(b(x_1+x_2)\right)\right)dt+\sqrt{\hbar}dw,$$

$$dx_2=\left(-x_2-a\sin\left(b(x_1+x_2)\right)\right)dt+\sqrt{\hbar}dw$$

with initial conditions $x_1(s)=x_{10}$, $x_2(s)=x_{20}$.

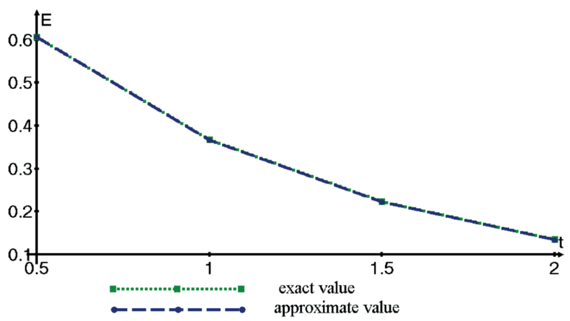

Fig. 1. Approximate and exact values of E, $\hbar=1$

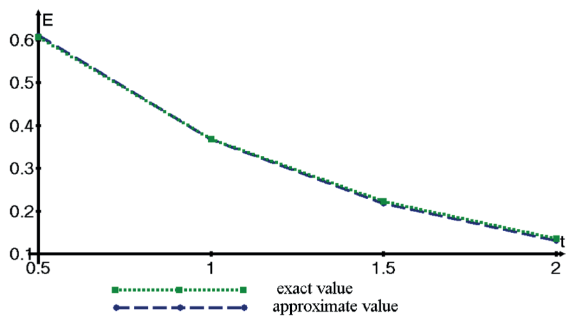

Fig. 2. Approximate and exact values of E, $\hbar=0.1$

For the mathematical expectation, the following equality is true:

$$E(x_1 - x_2) = (x_{10} - x_{20})\exp(-t).$$

From the numerical results shown in Figures 1 and 2, it can be seen that the semiclassical approximation well approximates the functional integral for various values of $\hbar$.

Thus, a numerical analysis of the accuracy of the semiclassical approximation of multiple functional integrals has been carried out in this work. For numerical analysis, we used a comparison of approximate values obtained using semiclassical approximation with exact values. The performed numerical analysis shows that the semiclassical approximation approximates well the functional integral for various values of $\hbar$.

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