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SIMPLE APPLICATIONS OF STATIONARY PATH INTEGRALS

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The practical use of the formalism presented previously is demonstrated by two simple one-dimensional examples (the square potential well and the WKB solution). The wave functions and energies of bound states are obtained in a very simple way mainly in the case of the WKB approximation.

ПРОСТЫЕ ПРИМЕНЕНИЯ СТАЦИОНАРНЫХ ИНТЕГРАЛОВ ПО ТРАЕКТОРИЯМ

Практическое использование формализма, введённого раньше, продемонстрировано на двух одномерных примерах (потенциальная яма и квазиклассическое решение). Волновые функции и энергии основных состояний получаются очень просто прежде всего в случае ВКБ – приближения.

I. INTRODUCTION AND METHOD

Firstly we shall briefly outline the stationary path integrals formalism. In [1] we showed that the solution of the equation

$$\left[\frac{d^2}{dx^2}+k^2(x)\right]\Psi(x)=0 \tag{1}$$

can be written in the following form

$$\Psi(x)=\sum_s A(s)k|x,a)\Psi_a^{(+)}+\sum_s A(s|k|x,b)\Psi_b^{(-)} \tag{2}$$

where $x\in\langle a,b\rangle$ and $A(s|k|x,a)$ is the amplitude of the trajectory s connecting the points a and x (it can be interpreted as the transition probability amplitude of the particle from a to x). The summation in Eq. (2) must be performed over all trajectories which connect the points in question and do not leave the interval $\langle a,b\rangle$. $\Psi_a^{(+)}$ and $\Psi_b^{(-)}$ are constant.

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If we replace $k(x)$ by

$$k_\varepsilon(x)=k(a+n\varepsilon) \quad \text{for} \quad x\in\langle a+n\varepsilon,\, a+(n+1)\varepsilon\rangle \tag{3}$$
$$n=0,1,\dots(N-1); \quad \varepsilon=(b-a)/N$$

then the amplitude of the trajectory s has this form

$$A(s|k_\varepsilon|x,a)=a(s|k_\varepsilon)\exp\left[\mathrm{i}\textstyle\int_s k_\varepsilon(x')\,\mathrm{d}l\right] \tag{4}$$

where $\mathrm{d}l$ is the element of length and the integral in the exponent is calculated along s. We note that in this case we consider only such trajectories the turning points of which are only the points $x_n=a+n\varepsilon$ (the turning point of s is such a point at which the particle changes the direction of its motion). The number $a(s|k_\varepsilon)$ is constructed in the following way:

i) we assign to the turning point $x_n=a+n\varepsilon$ the number

$$\pm\frac{k(x_{n-1})-k(x_n)}{k(x_{n-1})+k(x_n)},$$

ii) we assign to the transition of the trajectory s through the point $x_n=a+n\varepsilon$ the number

$$1\pm\frac{k(x_{n-1})-k(x_n)}{k(x_{n-1})+k(x_n)},$$

where the sign $+$ $(-)$ is taken at the time when the particle comes to x_n from the left (right). Then $a(s|k_\varepsilon)$ is equal to the product of all such numbers which must be taken into account for a given trajectory.

In the limit $\varepsilon\to0$ the amplitude of the trajectory, which has no turning point and connects the points a and x or b and x, is equal to

$$A(s_0|k|x,a)=\sqrt{\frac{k(a)}{k(x)}}\exp\left[\mathrm{i}\int_a^x k(y)\,\mathrm{d}y\right] \tag{5}$$

or

$$A(s_0|k|x,b)=\sqrt{\frac{k(b)}{k(x)}}\exp\left[\mathrm{i}\int_x^b k(y)\,\mathrm{d}y\right]. \tag{5'}$$

The sum of all amplitudes, each of which has one turning point $x_1\in(x,b)$ and connects the points a and x, is equal to

$$\sum_{s_1} A(s_1|k|x,a)=\sqrt{\frac{k(a)}{k(x)}}\exp\left[\mathrm{i}\int_a^x k(y)\,\mathrm{d}y\right]\left(-\frac{1}{2}\right)\int_x^b \mathrm{d}x_1\,\frac{k'(x_1)}{k(x_1)}\times$$
$$\times\exp\left[q_i\int_x^{x_1} k(y)\,\mathrm{d}y\right]. \tag{6}$$

Likewise

$$\sum_{s_1} A(s|k|x,b)=\sqrt{\frac{k(b)}{k(x)}}\exp\left[\mathrm{i}\int_x^b k(y)\,\mathrm{d}y\right]\left(+\frac{1}{2}\right)\int_a^x \mathrm{d}x_1\,\frac{k'(x_1)}{k(x_1)}\times$$
$$\times\exp\left[2\mathrm{i}\int_{x_1}^x k(y)\,\mathrm{d}y\right] \quad (k'(x)=\mathrm{d}k(x)/\mathrm{d}x) \tag{7}$$

is the sum of all amplitudes each of which has one turning point $x_1\in(a,x)$.

These results allow us to determine the amplitude of any trajectory. In what follows this formalism will be applied to two simple examples.

II. BOUND STATES

Let us now consider particles which are scattered by the potential

$$V(x)=\begin{cases} V_0=\text{const} & x<0\\ 0 & 0\leqslant x\leqslant b\\ \infty & x>b\end{cases} \tag{8}$$

and let the particle before the scattering be described by the amplitude $\Psi_{\text{in}}^{(+)}(x)=$ $=\exp[\mathrm{i}x\sqrt{E+\mathrm{i}0-V_0}]$ The solution of Eq. (1) for our case and for $x\in\langle0,b\rangle$ be equal to

$$\Psi(x)=\sum_s A(s|k|x,a)\,\Psi_{\text{in}}^{(+)}(a) \qquad (a<0). \tag{9}$$

The nonzero amplitudes are only those the turning points of which are only the points $x=0$ and $x=b$. In accordance with the formalism we assign i) to the turning point $x=b$ the number $R_b=-1$ and to $x=0$ the number $R_0=(k-k_0)/(k+k_0)$ (the particle comes to $x=0$ from the right) ii) to the transition of the trajectory through the point $x=0$ the number

$$\frac{2k}{k+k_0}\left(\frac{2k_0}{k+k_0}\right)$$

if the particle comes to $x=0$ from the left (right) where $k_0=(E+\mathrm{i}0)^{1/2}$ and $k=(E+\mathrm{i}0-V_0)^{1/2}$.

Then

$$\Psi^{(x)}_{0\leqslant x\leqslant b}=\Psi_{\text{in}}^{(+)}(a)\left[\mathrm{e}^{\mathrm{i}k_0x}\frac{2k}{k+k_0}\mathrm{e}^{-\mathrm{i}ka}+\right. \tag{10}$$
$$+\mathrm{e}^{\mathrm{i}k_0(b-x)}R_b\,\mathrm{e}^{\mathrm{i}k_0b}\frac{2k}{k+k_0}\mathrm{e}^{-\mathrm{i}ka}+$$

$$+\,\mathrm{e}^{\mathrm{i}k_0 x} R_0\, \mathrm{e}^{\mathrm{i}k_0 b} R_b\, \mathrm{e}^{\mathrm{i}k_0 b} \frac{2k}{k+k_0}\, \mathrm{e}^{-\mathrm{i}ka} + \dots \Big] .$$

The first term in the square bracket is the amplitude of the trajectory which has no turning point ($a \to 0 \to x$), the second term corresponds to the trajectory which has one turning point $x = b$ ($a \to 0 \to b \to x$), the third term corresponds to the trajectory ($a \to 0 \to b \to 0 \to x$), ...

The series in Eq. (10) can easily be summed. The result is

$$\Psi(x) = \Psi_{\mathrm{in}}^{(+)}(0)\, \frac{2k}{k+k_0}\, \frac{\mathrm{e}^{\mathrm{i}k_0 x} - \mathrm{e}^{2\mathrm{i}k_0 b}\, \mathrm{e}^{-\mathrm{i}k_0 x}}{1 + \dfrac{k_0 - k}{k_0 + k}\, \mathrm{e}^{2\mathrm{i}k_0 b}} . \tag{11}$$

The right-hand side of Eq. (10) as the function of E is singular at the points which satisfy the equation

$$1 = \frac{k - k_0}{k + k_0}\, \mathrm{e}^{2\mathrm{i}k_0 b} . \tag{12}$$

It is well known that these singularities are poles and their positions on the real E-axis determine the energy spectrum of the bound states. The bound state wave function is proportional to the residuum of $\Psi(x)$ at the corresponding pole.

Let us now consider the limit $V_0 \to \infty$. It follows from Eq. (10) (we do not write an unimportant factor) that

$$\Psi(x) \sim \Psi_{\mathrm{in}}^{(+)}(0)\, \frac{\sin k_0(x-b)}{\sin k_0 b} = \Psi_{\mathrm{in}}^{(+)}(0)\, \frac{\sin k_0(x-b)}{k_0 b \prod_{n=1}^{\infty} \left(1 - \dfrac{k_0^2 b^2}{n^2 \pi^2}\right)}$$

and on the basis of the foregoing we immediately obtain the solution of our problem.

III. ONE-DIMENSIONAL WKB SOLUTION

We assume that

i) the equation $E = V(x)$ has at most two roots x_1 and $x_2 > x_1$ ($V'(x_1) < 0$, $V'(x_2) > 0$),

ii) the potential $V(x)$ is such that only amplitudes of such trajectories the turning points of which are only the points x_1 and x_2 contribute to the total amplitude.

The sum of amplitudes, one turning point of which is situated in the small vicinity Ω of the point x_2, contains the factor (the particle comes to x_2 from the left)

$$-\frac{1}{2} \int_{\Omega(x_2)} \mathrm{d}x\, \frac{k'(x)}{k(x)} \exp\left[2\mathrm{i} \int_x k(y)\,\mathrm{d}y\right] = \tag{13}$$

$$= -\frac{P}{2} \int_{\Omega(x_2)} \mathrm{d}x\, \frac{k'(x)}{k(x)} \exp\left[2\mathrm{i} \int_x k(y)\,\mathrm{d}y\right] - \frac{\mathrm{i}\pi}{4} \exp\left[2\mathrm{i} \int_{x_1} k(y)\,\mathrm{d}y\right]$$

where P denotes the principle part. Eq. (13) will become clearer if we realize that we can write $V(x) \approx E + V'(x_2)(x - x_2)$ for $x \in \Omega(x_2)$ and $k(x) = \sqrt{E + \mathrm{i}0 - V(x)}$.

Likewise for the point x_1 (the particle comes to x_1 from the right)

$$\frac{1}{2} \int_{\Omega(x_1)} \mathrm{d}x\, \frac{k'(x)}{k(x)} \exp\left[2\mathrm{i} \int_x k(y)\,\mathrm{d}y\right] = \tag{14}$$

$$= \frac{P}{2} \int_{\Omega(x_2)} \mathrm{d}x\, \frac{k'(x)}{k(x)} \exp\left[2\mathrm{i} \int_x k(y)\,\mathrm{d}y\right] - \frac{\mathrm{i}\pi}{4} \exp\left[2\mathrm{i} \int_{x_1} k(y)\,\mathrm{d}y\right] .$$

It follows from (13—14) that we have to assign to the classical turning points the number $R = -\mathrm{i}\pi/4$. Then we obtain for the scattering amplitude the expression

$$\Psi(x) = \Psi_{\mathrm{in}}^{(+)}(a) \sqrt{\frac{k(a)}{k(x)}} \exp\left[\mathrm{i} \int_a^{x_1} k(y)\,\mathrm{d}y\right] \times \tag{15}$$

$$\times \frac{\exp\left[\mathrm{i} \int_{x_1}^{x} k(y)\,\mathrm{d}y\right] + R \exp\left[2\mathrm{i} \int_{x_1}^{x_2} k(y)\,\mathrm{d}y\right] \exp\left[-\mathrm{i} \int_{x_1}^{x} k(y)\,\mathrm{d}y\right]}{1 - R^2 \exp\left[2\mathrm{i} \int_{x_1}^{x_2} k(y)\,\mathrm{d}y\right]}$$

for $a < x_1 \leqslant x \leqslant x_2$

$$\Psi(x) = \Psi_{\mathrm{in}}^{(+)}(a) \sqrt{\frac{k(a)}{k(x)}} \exp\left[\mathrm{i} \int_a^{x_1} k(y)\,\mathrm{d}y\right] \times \tag{16}$$

$$\times \frac{\exp\left[\mathrm{i} \int_{x_1}^{x_2} k(y)\,\mathrm{d}y\right] \exp\left[-\int_{x_2}^{x} |k(y)|\,\mathrm{d}y\right]}{1 - R^2 \exp\left[2\mathrm{i} \int_{x_1}^{x_2} k(y)\,\mathrm{d}y\right]}$$

for $x \geqslant x_2$.

In what follows we put $R \approx -\mathrm{i}$. Then we obtain for the energies of the bound states the equation

$$\int_{x_1}^{x_2} k(x)\,\mathrm{d}x = \pi \left(n + \frac{1}{2}\right) \tag{17}$$

where $n = 0, 1, 2, \dots$ and for the wave functions the following expressions

$$\Psi^{(n)}_{x_1 \leqslant x \leqslant x_2} = \frac{2C_n}{\sqrt{k_n(x)}} \sin\left[\int_{x_1}^{x} k_n(y)\,\mathrm{d}y + \frac{\pi}{4}\right] \tag{18}$$

$$\Psi^{(x)}_{x'' \geq x_2} = \frac{(-1)^n C_n}{\sqrt{|k_n(x)|}} \exp\left[-\int_{x_2}^{x} |k_n(y)|\, dy\right] \tag{19}$$

where $k_n^2(x) = E_n - V(x)$ (E_n is the solution of Eq. (17)) and we formally put C_n to be proportional to "the residuum at the pole $E = E_n$" (it is not evident if the singularities in question are the poles in the case of the approximate amplitude (15—16)) of the function $\Psi_{in}^{(+)}(a)\, \sqrt{k(a)}\, e^{i\pi/4} \exp[i \int_a^{x_1} k(y)\, dy] \times (1 + \exp[2i \int_{x_1}^{x_2} k(y)\, dy])^{-1}$.

IV. CONCLUSION

In the foregoing sections we tried to outline how to solve some quantum mechanical examples by means of the stationary path integral formalism. The aim of this paper is to make clear the possibility of the practical use of the formalism.

In [1] we showed the equivalency (in the sense mentioned there) between the stationary path integrals and the integral representation of the Schrödinger equation presented by Baird [2] and therefore further applications can be found in [2], too.

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