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STATIONARY PATH INTEGRALS FORMALISM FOR THE ONE-DIMENSIONAL TIME-INDEPENDENT SCHRÖDINGER EQUATION

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We present the so-called stationary path integrals formalism for the one-dimensional time-independent Schrödinger equation. The conceptual framework of our formalism is almost the same as the one used by Feynman [1—2] in his formulation of quantum mechanics. The connection between the solution of the time-independent one-dimensional Schrödinger equation and boundary conditions (the values of the wave function are given at two different points) is given in a simple way by means of the so-called transition probability amplitudes of particles along trajectories.

ФОРМАЛИЗМ СТАЦИОНАРНЫХ ИНТЕГРАЛОВ ПО ТРАЕКТОРИЯМ ДЛЯ ОДНОМЕРНОГО УРАВНЕНИЯ ШРЕДИНГЕРА, НЕ ЗАВИСЯЩЕГО ОТ ВРЕМЕНИ

В статье рассматривается формализм так называемых стационарных интегралов по траекториям для одномерного уравнения Шредингера, не зависящего от времени. Схема данного формализма аналогична схеме формализма, который использовал Фейнман [1,2] в своей формулировке квантовой механики. Приводится простая связь между решением одномерного уравнения Шредингера, не зависящего от времени, и граничными условиями (значения волновой функции даются в двух разных точках) при помощи так называемой амплитуды вероятности перехода частицы вдоль траекторий.

I. MOTIVATION

In order to have a transparent picture of the problem (and we shall need in some sense this transparency below) we shall start with the following simple example. Let particles, having the energy $E > V_0 = \text{const}$, come from the left to the potential barrier

$$V(x) = V_0 \Theta(x - x_0)$$

($\Theta(x) = 1$ if $x > 0$ and $\Theta(x) = 0$ if $x < 0$) and let incident particles be described by the amplitude

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$$\Psi_{in}^{(+)}(x)=\exp(ik_0x),$$

where $k_0=+\sqrt{E}$ and we put $\hbar^2/2m=1$. The amplitude, describing this scattering, satisfies the equation

$$\left[\frac{d^2}{dx^2}-E-V_0\Theta(x-x_0)\right]\Psi(x)=0. \tag{1}$$

The solution of Eq. (1), corresponding to our case, is

$$\Psi(x)=e^{ik_0(x-a)}\Psi_{in}^{(+)}(a)+e^{ik_0(x_0-a)}\frac{k_0-k}{k_0+k}e^{ik_0(x_0-a)}\Psi_{in}^{(+)}(a), \tag{2}$$

for $a\leqslant x\leqslant x_O$ and

$$\Psi(x)=e^{ik(x-x_0)}\frac{2k_0}{k_0+k}e^{ik_0(x_0-a)}\Psi_{in}^{(+)}(a) \tag{3}$$

for $x\geqslant x_0$ $(k=+\sqrt{E-V_0})$.

The second term in (2) is interpreted as the amplitude describing particles which were reflected at the point x_0 (changed the sign of their momentum) back into the region $x<x_0$ and (3) represents the amplitude describing particles which penetrated into the region $x>x_0$.

Let us now consider the potentials of this type

$$V(x)=V_0\Theta(x-x_0)+V_1\Theta(x-x_1)+\ldots+V_N\Theta(x-x_N). \tag{4}$$

The phenomenon, described by the expressions (2—3) occurs any time when the incident particles appear in one of the points $x_0, x_1, \ldots, x_N$. Amplitudes describing particles which passed around a given point of a discontinuity of the potential (4) or reversed the direction of their momentum at this point can be calculated by means of the simple rules following from (2—3). In this way, we can, at least in principle, solve the problem of the scattering of particles on the potentials of the type (4). We note that this procedure can be used only in the case when E is not equal to $V(x)$ on any interval $\langle x_n, x_{n+1}\rangle$. We shall comment on the removing of this difficulty later on. Because "almost every" potential can be regarded as a limit of a sequence of potentials of type (4), the procedure outlined above indicates the possibility of an interesting method of finding solutions of some quantum mechanical problems.

II. THE TRANSITION PROBABILITY AMPLITUDE OF A PARTICLE FROM THE POINT $x=0$ INTO THE POINT $x=a$ ALONG THE TRAJECTORY s

For the sake of simplicity, let us choose the uniform partition of the coordinate axis x and replace the function $k(x)=+(E-V(x))^{1/2}$ by an approximate function

$$k_\varepsilon(x)=k(n\varepsilon) \quad \text{for} \quad x\in\langle n\varepsilon,(n+1)\varepsilon\rangle \tag{5}$$
$$n=0,\pm1,\pm2,\ldots$$

We assume that $V(x)$ is continuous and $V(x)<E$. The more general case will be considered later on (the end of Sec. IV.).

Let us now consider continuous trajectories connecting the points $x=0$ and $x=a$. Let the point x_n be situated on the trajectory s. We shall say that the point x_n is a turning point of s if the particle which moves along s from $x=0$ to $x=a$ approaches x_n from the left (right) and leaves x_n in the direction to the left (right). If x_n is not a turning point of s, then we shall say that the particle (or the trajectory) passes through x_n or x_n is one of the points $x=0$ and $x=a$.

In what follows we shall consider only such trajectories the turning points of which are only the points $x_n=n\varepsilon$, where n is an integer. In this case we assign to the trajectory s the amplitude

$$A(s|k_\varepsilon|a,0)=a(s|k_\varepsilon)\exp(i\textstyle\int_s dlk_\varepsilon(x)), \tag{6}$$

where dl is an element of the length s and $\int_s dl$ means an integral along s. The number $a(s|k_\varepsilon)$ is constructed in the following way:

i) We assign to the turning point $x_n\in s$ the number $(k(x_{n-1})-k(x_n))/(k(x_{n-1})+k(x_n))$ if the particle comes to x_n from the left or the number $(k(x_n)-k(x_{n-1}))/(k(x_n)+k(x_{n-1}))$ if the particle comes to x_n from the right;

ii) We assign to the transition of the particle (or the trajectory) through the point $x_n=n\varepsilon$ (n is an integer) the number $2k(x_{n-1})/(k(x_n)+k(x_{n-1}))$ if the particle comes to x_n from the left or the number $2k(x_n)/(k(x_n)+k(x_{n-1}))$ if the particle comes to x_n from the right;

then $a(s|k\varepsilon)$ is equal to the product of all such numbers which must be taken into account for the trajectory s. If s has no turning point and does not pass through any $x_n=n\varepsilon$, then $a(s|k_\varepsilon)=1$.

One can see (taking into account (2—3)) that $A(s|k_\varepsilon|a,0)$ can indeed be interpreted as the transition probability amplitude of the particle from $x=0$ to $x=a$ along s. In what follows (6) will be simply called the amplitude of the trajectory s.

III. THE SOLUTION OF THE SCHRÖDINGER EQUATION IN TERMS OF THE AMPLITUDES OF TRAJECTORIES

Let us seek the solution of the equation

$$\left[\frac{d^2}{dx^2}+k_\varepsilon^2(x)\right]\varphi_\varepsilon(x)=0 \tag{7}$$

on the interval $\langle 0, a\rangle$ with the boundary conditions

$$\varphi_\varepsilon(0)=\Psi_0 \qquad \varphi_\varepsilon(a)=\Psi_a\,. \tag{8}$$

It is evident that for any $x\in\langle 0, a\rangle$ the solution of Eq. (7) can be written in the form

$$\varphi_\varepsilon(x)=\varphi_\varepsilon^{(+)}(x)+\varphi_\varepsilon^{(-)}(x), \tag{9}$$

where $\varphi_\varepsilon^{(+)}(x)$ ($\varphi_\varepsilon^{(-)}(x)$) represents the amplitude describing particles moving from the left (right) to the right (left).

On the basis of the previous result we can write $\varphi_\varepsilon(x)$ in the following form

$$\varphi_\varepsilon(x)=\sum_s A(s|k_\varepsilon|x, 0)\,\Psi_0^{(+)}+\sum_s A(s|k_\varepsilon|x, a)\,\Psi_a^{(-)}, \tag{10}$$

where $\Psi_0^{(+)}=\varphi_\varepsilon^{(+)}(0)$, $\Psi_a^{(-)}=\varphi_\varepsilon^{(-)}(a)$, $\sum_s$ means the summation over all possible trajectories which connect the points 0 and x or a and x, do not come out of the interval $\langle 0, a\rangle$ and have the turning points only at $x_n=n\varepsilon$ ($n=1, 2, \ldots, N-1$ if $a=N\varepsilon$).

Equation (10) will be more transparent if we realize that for $\Psi_a^{(+)}$ to contribute to $\varphi_\varepsilon(x)$ it is necessary that particles which start from $x=a$ in the positive direction of the axis x reflect somewhere to the right and then pass through the point $x=a$. However, this effect is already included in $\Psi_a^{(-)}$. And that is why $\Psi_0^{(-)}$ does not occur in (10), too. From this it follows that for $\Psi_0^{(-)}$ and $\Psi_a^{(+)}$ we have to write the following equations

$$\Psi_0^{(-)}=\sum_s A(s|k_\varepsilon|0, 0)\,\Psi_0^{(+)}+\sum_s A(s|k_\varepsilon|0, a)\,\Psi_a^{(-)}, \tag{11}$$

$$\Psi_a^{(+)}=\sum_s A(s|k_\varepsilon|a, 0)\,\Psi_0^{(+)}+\sum_s A(s|k_\varepsilon|a, a)\,\Psi_a^{(-)}. \tag{12}$$

Eqs. (11, 12) together with equations which we obtain from (9) by substituting into (9) successively $x=0$ and $x=a$ allow us to calculate $\Psi_0^{(\pm)}$ and $\Psi_a^{(\pm)}$.

Having realized that

$$\lim_{x\to 0^+}\sum_s A(s|k_\varepsilon|x, 0)=1+\sum_s A(s|k_\varepsilon|0, 0)$$

$$\lim_{x\to a^-}\sum_s A(s|k_\varepsilon|x, a)=1+\sum_s A(s|k_\varepsilon|a, a),$$

it is not difficult to show that $\varphi_\varepsilon(x)$ given by (10) fulfils the desired boundary conditions and if we take into account that the continuity conditions for $\varphi_\varepsilon(x)$ and its derivative are satisfied in the way by which we assigned $A(s|k_\varepsilon|\ldots)$ to the trajectory s, then (10) is indeed the desired solution of our problem (of course, if the solutions of Eqs. (11, 12) and equations obtained from (9) exist).

IV. FORMAL LIMIT $\varepsilon\to 0$

Leaving aside the problems connected with the limit $\varepsilon\to 0$ let us now investigate this limit only from the formal point of view. We assume that $k(x)$ is differentiable on intervals considered below. Let us now consider the trajectory s_0, which has no turning points and which connects the points x_0 and $x>x_0$. In Sec. II. we assigned to s_0 the amplitude

$$A(s_0|k|x, x_0)=\lim_{\varepsilon\to 0} a(s_0|k_\varepsilon)\,e^{i\int_{x_0}^{x}k(y)dy}, \tag{13}$$

where

$$a(s_0|k_\varepsilon)=\prod_n\frac{2k(x_{n-1})}{k(x_n)+k(x_{n-1})}=\prod_n\left(1-\frac{k(x_n)-k(x_{n-1})}{k(x_n)+k(x_{n-1})}\right)$$

(n is an integer and runs over the corresponding set of indices). For a sufficiently small ε we can write

$$a(s_0|k_\varepsilon)\approx\prod_n\left(1-\frac{k'(x_n)}{2k(x_n)}\varepsilon\right).$$

Then

$$\lim_{\varepsilon\to 0} a(s_0|k_\varepsilon)=e^{-\frac{1}{2}\int_{x_0}^{x}\frac{k'(y)}{k(y)}dy}=\sqrt{\frac{k(x_0)}{k(x)}}, \tag{14}$$

where $k'(y)=dk(y)/dy$ and

$$A(s_0|k|x, x_0)=\sqrt{\frac{k(x_0)}{k(x)}}\,e^{i\int_{x_0}^{x}k(y)dy}. \tag{15}$$

Let us further consider the sum of amplitudes of trajectories each of which has only one turning point. Let the trajectories again connect the points x_0 and $x>x_0$ and the corresponding turning points are situated in the interval $\langle a, b\rangle$ ($x_0<x<a<b$). The sum of all such amplitudes is

$$\sum_{s_1}A(s_1|k|x, x_0)=\lim_{\varepsilon\to 0}\sum_n A(s_0|k_\varepsilon|x, x_n)\left(-\frac{1}{2}\right)\frac{k'(x_n)}{k(x_n)}\varepsilon\times$$
$$\times A(s_0|k_\varepsilon|x_n, x_0).$$

If we take into account that

$$A(s_0|k|x, x_n)\,A(s_0|k|x_n, x)=e^{2i\int_{x}^{x_n}k(y)dy},$$

then

$$\sum_{s_1} A(s_1|k|x, x_0) = \sqrt{\frac{k(x_0)}{k(x)}}\, e^{i\int_{x_0}^{x} k(y)dy} \times$$

$$\times\left(-\frac{1}{2}\right)\int_a^b dx_1 \frac{k'(x_1)}{k(x_1)} e^{2i\int_x^{x_1} k(y)dy}. \quad (16)$$

We obtain likewise for the sum of amplitudes of trajectories each of which has only one turning point in $\langle c, d\rangle$ $(c<d<x_0<x)$

$$\sum_{s_1} A(s_1|k|x, x_0) = \sqrt{\frac{k(x_0)}{k(x)}}\, e^{i\int_{x_0}^{x} k(y)dy} \times$$

$$\times\left(\frac{1}{2}\right)\int_c^d dx_1 \frac{k'(x_1)}{k(x_1)} e^{2i\int_{x_1}^{x_0} k(y)dy}. \quad (17)$$

These results allow us to write in a compact form the sum of amplitudes belonging to the given class of trajectories.

As an illustration we present the following example. Let incident particles be scattered by the potential $V(x)$ $(V(x)\to 0$ if $|x|\to\infty)$ and let these particles be described before their scattering by the amplitude

$$\Psi_{in}^{(+)}(x) \xrightarrow[x\to-\infty]{} \exp(ix\sqrt{E}).$$

For the amplitude describing this scattering we write

$$\Psi(x) = \lim_{a\to-\infty} \Psi_{in}^{(+)}(a)\sqrt{\frac{k(a)}{k(x)}}\, e^{i\int_a^x k(y)dy}\left[1-\frac{1}{2}\int_x^\infty dx_1 \frac{k'(x_1)}{k(x_1)} e^{2i\int_x^{x_1} k(y)dy} -\right.$$

$$-\frac{1}{4}\int_a^x dx_1 \frac{k'(x_1)}{k(x_1)}\int_{x_1}^\infty dx_2 \frac{k'(x_2)}{k(x_2)}\times \quad (18)$$

$$\times e^{2i\int_{x_1}^{x_2} k(y)dy} + \frac{1}{8}\int_x^\infty dx_3 \frac{k'(x_3)}{k(x_3)} e^{2i\int_x^{x_3} k(y)dy}\times$$

$$\left.\times\int_a^{x_3} dx_1 \frac{k'(x_1)}{k(x_1)}\int_{x_1}^\infty dx_2 \frac{k'(x_2)}{k(x_2)} e^{2i\int_{x_1}^{x_2} k(y)dy} + \ldots\right].$$

The third term in the squared bracket multiplied by the term standing in front of the bracket corresponds to the sum of amplitudes of all possible trajectories which connect the points in question, do not come out of the interval $\langle a, \infty)$ and have two turning points x_1 and $x_2>x_1$. The other terms in (18) have a similar meaning.

It is evident that, in general, the integrals in (18) are not unambiguously defined. It is necessary to give rules how to integrate over the interval containing the classical turning points $(E=V(x))$. The natural demand how to specify these rules is the requirement of the correct asymptotic behaviour of $\Psi(x)$. The correct asymptotic behaviour is obtained by the replacement of $E\to E+i0$.

V. CONCLUSION

In [1] Feynman introduced the notion of the transition probability amplitude of a particle from a (space-time) point $(\mathbf{x}_0, t_0)$ to a point $(\mathbf{x}_1, t_1)$ along the trajectory (history) $\mathbf{x}_s(t)$, where $\mathbf{x}_s(t_0)=\mathbf{x}_0$ and $\mathbf{x}_s(t)_1=\mathbf{x}_1$. The corresponding nonrelativistic amplitude of the spinless particle is according to [1] equal to

$$C e^{i\int_{t_0}^{t_1} dt L(\dot{\mathbf{x}}_s(t), \mathbf{x}_s(t), t)}, \quad (19)$$

where L is the Lagrange function of the considered particle and the constant C does not depend on the form (geometry) and character (time-develompment) of $\mathbf{x}_s(t)$. The total transition probability amplitude of the particle from $(\mathbf{x}_0, t_0)$ to $(\mathbf{x}_1, t_1)$ is equal to the sum of amplitudes of all possible trajectories connecting to points in question. For mathematical details the reader is referred to [1, 2].

If the wave function is defined in such a way that

$$\psi(\mathbf{x}_1, t_1) = \int d\mathbf{x}_0 C\sum_s e^{i\int_{t_0}^{t_1} dtL}\ \Psi(\mathbf{x}_0, t_0), \quad (20)$$

then one can show [1, 2] that this formulation of quantum mechanics is equivalent to the Schrödinger formulation. From this point of view Eq. (10) can be considered as an analogon of Eq. (20). Eq. (10) directly connects (in the spirit of the path integrals formalism mentioned above) boundary conditions with the solution of eq. (7). The interpretation of mathematical expressions in (10) is as simple and transparent as in the case of Eq. (20).

In [3] Baird presented an interesting integral formulation of the one-dimensional time independent Schrödinger equation. He sought the solution (on the interval $\langle a, b\rangle$) in the form

$$\Psi(x) = \frac{1}{\sqrt{k(x)}} e^{i\int_a^x k(y)dy}\ \varkappa^{(+)}(x) + \frac{1}{\sqrt{k(x)}} e^{-i\int_a^x k(y)dy}\ \varkappa^{(-)}(x) \quad (21)$$

and he derived for $\varkappa^{(\pm)}(x)$ the following integral equations

$$\varkappa^{(+)}(x) = A^{(+)} + \int_a^x \mathrm{d}x_1 \frac{k'(x)_1}{2k(x_1)} \mathrm{e}^{-2\mathrm{i}\int_a^{x_1} k(y)\mathrm{d}y} \varkappa^{(-)}(x_1), \tag{22}$$

$$\varkappa^{(-)}(x) = A^{(-)} - \int_x^b \mathrm{d}x_1 \frac{k'(x_1)}{2k(x_1)} \mathrm{e}^{2\mathrm{i}\int_a^{x_1} k(y)\mathrm{d}y} \varkappa^{(+)}(x_1), \tag{23}$$

where $A^{(\pm)}$ are constants.

If we solve these equations by an iterative method (the zero approximations are $\varkappa_0^{(\pm)}(x) = A^{(\pm)}$), then the individual terms of the expansion have, at first sight, the same mathematical structure as the amplitudes of trajectories connecting the points a and x *or* b and x. Naturally there arises the question whether our formalism is equivalent to Eqs. (21—23). The equivalency (in the sense mentioned above) can be proved for example by the mathematical induction method (we put $A^{(+)} = \sqrt{k(a)}\,\Psi_a^{(+)}$ and $A^{(-)} = \sqrt{k(b)}\,\Psi_b^{(-)} \exp(\mathrm{i}\int_a^b k(y)\,\mathrm{d}y)$). The proof is simply but somewhat lenghty and we shall therefore not present it here.

Although the stationary path integral formalism does not increase the number of exactly soluable problems in quantum mechanics yet it forms a basis for an unconventional approach to some simple problem and perhaps its further development can lead to some effective approximation method. The generalization of the formalism presented above for a three dimensional case is not, it seems to us, trivial but it turns out that it can be used for the radial Schrödinger equation.

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