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WAVE FUNCTIONS OF THE LEFT AND RIGHT SCATTERING PROBLEMS AS A BASIS FOR DESCRIPTION OF A WAVE PROCESS EVOLUTION

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We show that in Hilbert space the wave functions corresponding to different scattering problems are orthogonal with respect to each other for any potential. We prove that a wave process which propagates in a space symmetrically can be excited in the case of a symmetric potential only, when the spectral compositions of the left and right scattering functions generating a wave packet coincide with each other.

Keywords: left and right scattering problems, wave process evolution

1. Introduction

It this work we investigate some properties of a one-dimensional non-stationary motion, which is performed on the base of the stationarymotion consideration. It is well known that any one-dimensional quantum mechanics motion of stationary character is described by one-dimensional Schrodinger equation:

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

where $k=\sqrt{2mE}/\hbar$, $u(x)=2mU(x)/\hbar^2$ and E, $U(x)$ are total and potential energies.

Further we will suppose that $U(x)$ tends to zero, when $x\to\pm\infty$, so that the asymptotic form of an arbitrary solution of Eq. (1) can be written:

$$\Psi(x,k)=\begin{cases} a\exp\{ikx\}+b(k)\exp\{-ikx\}, & x\to-\infty,\\ c(k)\exp\{ikx\}+d\exp\{-ikx\}, & x\to+\infty. \end{cases} \tag{2}$$

Here we explicitly mark the solution dependence on the parameter k. Note that when $k>0$ the quantities a, d are being the amplitudes of the waves converging to a potential and b, c are the amplitudes of the diverging waves. In Eq. (2) we suggest that the amplitudes of the converging waves are initially given quantities, therefore the amplitudes of the diverging waves depend on the parameter k.

The connection between the wave amplitudes propagating in left and right sides of a potential is given by the transfer matrix [1-3];

$$\begin{pmatrix} c(k) \\ d \end{pmatrix} = \begin{pmatrix} \alpha(k) & \beta(k) \\ \beta(-k) & \alpha(-k) \end{pmatrix} \begin{pmatrix} a \\ b(k) \end{pmatrix}, \qquad (3)$$

where $\alpha(k)\alpha(-k) - \beta(k)\beta(-k) = 1$. By using Eq. (3) it is easy to check that the asymptotic behavior of the function $\Psi(x,-k)$ obtained from $\Psi(x,k)$ by change the sign of the parameter k has the following asymptotic behavior:

$$\Psi(x,-k) = \begin{cases} a\exp\{-ikx\} + b(-k)\exp\{ikx\}, & x \to -\infty, \\ c(-k)\exp\{-ikx\} + d\exp\{ikx\}, & x \to +\infty. \end{cases} \qquad (4)$$

Note that the function $\Psi(x,-k)$ is a solution of Eq. (1) as well, but in contrast to solution $\Psi(x,k)$ here the initially given constants a, d correspond to the amplitudes of the diverging waves. For the solution $\Psi(x,-k)$ a connection between the amplitudes rewritten by means of the transfer matrix has the form

$$\begin{pmatrix} d \\ c(-k) \end{pmatrix} = \begin{pmatrix} \alpha(k) & \beta(k) \\ \beta(-k) & \alpha(-k) \end{pmatrix} \begin{pmatrix} b(-k) \\ a \end{pmatrix}. \qquad (5)$$

It is easy to check that Eq. (3) and Eq. (5) are equivalent.

2. Some properties of the wave functions of the left and right scattering problems

If one takes $a = 1$, $d = 0$ (a wave falls on potential from its left side and there is no wave falling on a barrier from the right side), then $c = T(k)$, $b = R(k)$ and the wave function $\Psi_k(x)$ of the asymptotic behavior Eq.(2) will describe or correspond to the left scattering problem:

$$\Psi_{left}(x,k) = \frac{1}{\sqrt{2\pi}} \begin{cases} \exp\{ikx\} + R(k)\exp\{-ikx\}, & x \to -\infty, \\ T(k)\exp\{ikx\}, & x \to +\infty, \end{cases} \qquad (6)$$

where $T(k)$ and $R(k)$ are the transmission and reflection amplitudes of the left scattering problem.

For the right scattering problem a wave falls on a potential from its right side only and there is no wave falling on the barrier from its left side, i.e. $a = 0$, $d = 1$ and $c = P(k)$, $b = S(k)$ and

$$\Psi_{right}(x,k) = \frac{1}{\sqrt{2\pi}} \begin{cases} S(k)\exp\{-ikx\}, & x \to -\infty, \\ \exp\{-ikx\} + P(k)\exp\{ikx\}, & x \to +\infty, \end{cases} \qquad (7)$$

where $S(k)$, $P(k)$ are the transmission and reflection amplitudes of the right scattering problem.

Note that in Eq. (6) and Eq. (7) the factor $1/\sqrt{2\pi}$ provides the normalization conditionof the scattering wave functions (see, for example, [4]), which does not depend on the potential form:

$$\int_{-\infty}^{\infty} \Psi_{left}(x,k)\Psi_{left}(x,-k')\,dx = \delta(k-k'), \int_{-\infty}^{\infty} \Psi_{right}(x,k)\Psi_{right}(x,-k')\,dx = \delta(k-k'). \quad (8)$$

The functions $\Psi_{left}(x,k)$ and $\Psi_{right}(x,k)$ are linearly independent solutions of Eq. (1), so its arbitrary solution can be presented by those in a form of a linear combination.For the transmission and reflection amplitudes of the left and right scattering problems, the following relations take place[1-3]:

$$1 - R(k)R(-k) = T(k)T(-k), \quad (9)$$

$$1 - P(k)P(-k) = S(k)S(-k), \quad \backslash \quad (10)$$

$$P(k)T(-k) + R(-k)S(k) = 0, \; P(-k)T(k) + R(k)S(-k) = 0, \quad (11)$$

$$T(k) = S(k), \; T(-k) = S(-k). \quad (12)$$

The given equations are obtained by means of the transfer matrix (see Eq. (5)) written with the help of scattering amplitudes of the left and right scattering problems:

$$\begin{pmatrix} \alpha(k) & \beta(k) \\ \beta(-k) & \alpha(-k) \end{pmatrix} = \begin{pmatrix} \dfrac{1}{T(-k)} & \dfrac{-R(-k)}{T(-k)} \\ \dfrac{-R(k)}{S(k)} & \dfrac{1}{T(k)} \end{pmatrix} = \begin{pmatrix} \dfrac{1}{S(-k)} & \dfrac{P(k)}{S(k)} \\ \dfrac{P(-k)}{S(-k)} & \dfrac{1}{S(k)} \end{pmatrix}.$$

Note that for the case, when in Eq. (1) the potential $u(x)$ is a real function, theaction sign change of the parameter k is equivalent to the complex conjugation action (for example, $T(-k) = T^*(k)$, $R(-k) = R^*(k)$ and so on).Further we will discuss a real potential case, in which one can write

$$\Psi_{left}(x,-k) = \Psi^*_{left}(x,k), \; \Psi_{right}(x,-k) = \Psi^*_{right}(x,k). \quad (13)$$

If the orthogonality of the wave functions andconjugate functions for separate scattering problem can be seen easily, the same thing cannot be said for the wave functionscorrespondingto both scattering problems. However, to have the basis of functions containing simultaneously the scattering functions $\Psi_{left}(x,k)$, $\Psi_{right}(x,k)$ is very important, because it allows to substantiallyenlarge the class of wave processes possible to be considered.

3. The orthogonality of the wave functions of the left and right scattering problems

From the theoretical and practical point of view it is interesting to investigate how the wave functions $\Psi_{left}(x,k)$ and $\Psi_{right}(x,k)$ relate to each other in Hilbert space of wave functions of one-dimensional motion. This couple of functions is useful basis for consideration of evolution problem of nonstationary wave processes.So, in the framework of this basis a sufficiently wide class of wave process $\Phi(x,t)$ can be presented with expansion coefficients independent of time:

$$\Phi(x,t)=\int_0^{\infty}\left[v_{left}(k)\Psi_{left}(x,k)+v_{right}(k)\Psi_{right}(x,k)\right]\exp\{-iE(k)t/\hbar\}dk\,, \tag{14}$$

where $v_{left}(k)$, $v_{right}(k)$ are coefficients of the expansion spectrum conducted on the basis of the functions $\Psi_{left}(x,k)$, $\Psi_{right}(x,k)$ and $E(k)=\hbar^2k^2/2m$. Note that for any another basis, for example, the Fourier waves,

$$\frac{1}{\sqrt{2\pi}}\exp\{i(kx-E(k)t/\hbar)\},\quad \frac{1}{\sqrt{2\pi}}\exp\{-i(kx+E(k)t/\hbar)\}\,,$$

the expansion coefficients will be functions of t for the free wave motion:

$$\Phi(x,t)=\frac{1}{\sqrt{2\pi}}\int_0^{\infty}\left[\theta_+(k,t)\exp\{ikx\}+\theta_-(k,t)\exp\{-ikx\}\right]\exp\{-iE(k)t/\hbar\}dk\,,$$

where $\theta_+(k,t)$ and $\theta_-(k,t)$ are the expansion coefficients on the Fourier waves propagation in opposite directions.

Multiplying Eq. (14) by $\Psi^*_{left}(x,k)$ and integrating it over a space coordinate x and taking into account Eq. (8), Eq. (13), for the expansion coefficient $v_{left}(k)$ one can write

$$v_{left}(k)=\int_{-\infty}^{+\infty}\Phi_0(x)\Psi^*_{left}(x,k)dx-v_{right}(k)\int_{-\infty}^{+\infty}\Psi_{right}(x,k)\Psi^*_{left}(x,k)dx\,. \tag{15}$$

The coefficient $v_{right}(k)$ is analogously obtained from Eq. (14) by multiplying it by $\Psi_{right}(x,k)$:

$$v_{right}(k)=\int_{-\infty}^{+\infty}\Phi_0(x)\Psi^*_{right}(x,k)dx-v_{left}(k)\int_{-\infty}^{+\infty}\Psi_{left}(x,k)\Psi^*_{right}(x,k)dx\,, \tag{16}$$

where we denoted $\Phi(x,0)=\Phi_0(x)$, which is the initial form of a wave perturbation. In accordance to Eq. (14), the function $\Phi_0(x)$ is determined by means of the spectral coefficients:

$$\Phi_0(x)=\int_0^{\infty}\left[v_{left}(k)\Psi_{left}(x,k)+v_{right}(k)\Psi_{right}(x,k)\right]dk\,. \tag{17}$$

It is easy to see that last parts of Eq. (15) and Eq. (16) are expressed by integrals containing the product of functions $\Psi_{left}(x,-k)$, $\Psi_{right}(x,k)$ and $\Psi_{left}(x,k)$, $\Psi_{right}(x,-k)$.It is possible to show that in Hilbert space the wave functions of the left and right scattering problems are orthogonal always (see Appendix):

$$\int_{-\infty}^{+\infty} \Psi_{right}(x,k)\Psi^*_{left}(x,k)dx = \int_{-\infty}^{+\infty} \Psi_{left}(x,k)\Psi^*_{right}(x,k)dx = 0 . \tag{18}$$

In accordance with Eq. (17) for the expansion coefficient $v_{left}(k)$ and $v_{right}(k)$ Eq. (15), Eq. (16) is possible to present

$$v_{left}(k) = \int_{-\infty}^{+\infty} \Phi_0(x)\Psi^*_{left}(x,k)dx , \; v_{right}(k) = \int_{-\infty}^{+\infty} \Phi_0(x)\Psi^*_{right}(x,k)dx . \tag{19}$$

So, we proved that for an arbitrary one-dimensional field the wave functions of the left and right scattering problems are perpendicular in Hilbert space functions.

4. The evolution of the wave packet constructed on the base of wave functions of both scattering problems

Below we consider a wave packet involving the wave functions of both scattering problems (see Eq. (14)). Suppose that a process wave field is normalized, so that one can write down

$$\int_{-\infty}^{+\infty} \Phi(x,t)\Phi^*(x,t)dx = 1 . \tag{20}$$

Using Eq. (8), Eq. (18) for the spectral expansion coefficients of a wave process satisfying to this normalization condition, one can get

$$1 = \int_0^{\infty} \left[v_{left}(k)v^*_{left}(k) + v_{right}(k)v^*_{right}(k) \right] dk. \tag{21}$$

The initial conditions of excitation should be chosen such as for any time moment the wave permutation has a symmetric form: $\Phi(x,t) = \Phi(-x,t)$. In other words, the evolution of a wave packet should take place symmetrically with respect to the origin of coordinates. It is clear that it can be only in case when the function, describing the initial perturbation, is an even function: $\Phi_0(x) = \Phi_0(-x)$.

In accordance with Eq. (17), the function $\Phi_0(x)$ will be symmetric, only if the under-integral function is an even function as well:

$$\varphi(x,k)=\varphi(-x,k)\,, \tag{22}$$

where

$$\varphi(x,k)=v_{left}(k)\Psi_{left}(x,k)+v_{right}(k)\Psi_{right}(x,k)\,. \tag{23}$$

It is interesting to note that if one chooses the spectral compositions of the left and right scattering waves as being equal to each other,

$$v_{left}(k)=v_{right}(k)=v(k)\,, \tag{24}$$

It does not mean that Eq. (22) takes place automatically. As we see below, Eq. (22) can be satisfied when the equality

$$\Psi_{left}(x,k)=\Psi_{right}(-x,k) \tag{25}$$

takes place. Indeed, only in these cases the function $\varphi(x,k)$ (see Eq. (23), Eq. (24)) is even:

$$\varphi(x,k)=v(k)\Big[\Psi_{left}(x,k)+\Psi_{left}(-x,k)\Big]=v(k)\Big[\Psi_{right}(x,k)+\Psi_{right}(-x,k)\Big]\,. \tag{26}$$

Note that in accordance to Eq. (7) the function $\Psi_{right}(-x,k)$ has the asymptotic form coinciding with asymptotic behavior of $\Psi_{left}(x,k)$ (see Eq. (6)):

$$\Psi_{right}(-x,k)=\frac{1}{\sqrt{2\pi}}\begin{cases}\exp\{ikx\}+P(k)\exp\{-ikx\}, & x\to-\infty,\\ S(k)\exp\{ikx\}, & x\to+\infty.\end{cases} \tag{27}$$

It is clear that the amplitudes of the transmitted and reflected waves for the solutions $\Psi_{left}(x,k)$ and $\Psi_{right}(-x,k)$ should be equal to each other. Comparing Eq. (27) with Eq. (6), one can see that the equality (25) takes place if

$$T(k)=S(k)\ \text{ and }\ R(k)=P(k)\,. \tag{28}$$

The first equality of Eq. (28) takes place for any value of k (see Eq. (12)) and for any form of a potential. The second equality of Eq. (28) imposes a certain restriction on the form of potential values of k. Comparing Eq. (27) with Eq. (6) it is easy to see that the equality $R(k)=P(k)$ takes place only when the scattering potential has a symmetric form, namely $u(x)=u(-x)$.This result shows that a wave process which propagates symmetrically can be excited in the case of symmetric potential only, when the spectral compositions of the left andright scattering functions generating a wave packet coincide with each other.

5. Conclusion

In the scope of this article, we investigated the question of orthogonality of the scattering wave functions corresponding to the left and right scattering problems. We have shown that in

Hilbertspace, for any potential, the wave functions corresponding to different scattering problems are orthogonal with respect to each other. The basis includingboth scattering functions are very useful for investigation of a wave evolution process whichstarts itspropagation from a region inside the potential volume. For a case of symmetric potential, we found an analytical condition, when the symmetric wave process can be excited.

Appendix

By using Eq. (1) for any two solutions $\Psi_1(x,k)$ and $\Psi_2(x,k)$ one can write down (see, for example, [5–7]):

$$\int_{-L}^{L} \Psi_1(x,k)\Psi_2^*(x,k')dx = \frac{1}{k'^2-k^2}\left[\Psi_2^*(x,k')\frac{d\Psi_1(x,k)}{dx} - \Psi_1(x,k)\frac{d\Psi_2^*(x,k')}{dx}\right]\Bigg|_{-L}^{L}. \quad \text{(A.1)}$$

Considering large values of L for Eq. (A.1) one can write

$$\int_{-L}^{L} \Psi_1(x,k)\Psi_2^*(x,k')\,dx = f_1(k,k')\frac{\sin\{(k-k')L\}}{k-k'} + f_2(k,k')\frac{i\cos\{(k-k')L\}}{k-k'} + \\ + f_3(k,k')\frac{\sin\{(k+k')L\}}{k+k'} + f_4(k,k')\frac{i\cos\{(k+k')L\}}{k+k'}, \quad \text{(A.2)}$$

where

$$f_1(k,k') = a_1a_2 + d_1d_2 + c_2^*(k')c_1(k) + b_2^*(k')b_1(k)\,, \quad \text{(A.3)}$$

$$f_2(k,k') = a_1a_2 + d_1d_2 - c_2^*(k')c_1(k) - b_2^*(k')b_1(k)\,, \quad \text{(A.4)}$$

$$f_3(k,k') = a_1b_2^*(k') + d_1c_2^*(k') + a_2b_1(k) + d_2c_1(k)\,, \quad \text{(A.5)}$$

$$f_4(k,k') = a_1b_2^*(k') + d_1c_2^*(k') - a_2b_1(k) - d_2c_1(k) \quad \text{(A.6)}$$

and a_1, a_2, d_1, d_2 and $c_1(k)$, $c_2(k), b_1(k)$, $b_2(k)$ are the amplitudes on converging and diverging waves propagating on both sides of a potential.

When the quantities k and k' are treated as real values, then, as a function of L, the expression (A.2) includes oscillating factors of the following behavior:

$$\sin\{yL\}/y\ , \quad \cos\{yL\}/y, \quad \text{(A.7)}$$

where $y = k - k'$ or $y = k + k'$. Note that both expressions $\sin\{yL\}/y$ and $\cos\{yL\}/y$ as functions of y always tend to zero, under condition that $L \to \infty$ for all values of $y \neq 0$. The function $\sin\{yL\}/y$ is an even functionand in the limit $L \to \infty$ for the value $y = 0$ it tends to $+\infty$. The function $\cos\{yL\}/y$ is an odd function, which value is uncertain at $y = 0$, since the limits $y \to +0$ and $y \to -0$ are different for this function. For values $y \to +0$ the function $\cos\{yL\}/y$ tends to $+\infty$ and when $y \to -0$, it tends to $-\infty$.

The defined meaning for functions (A.7) can be given in the class of generalized functions. Considering $L \to \infty$ and taking $dy = dk$ for the summands of (A.2) difference, we obtain

$$\lim_{L\to\infty} \int_{-\infty}^{\infty} f_1(k,k') \frac{\sin\{(k-k')L\}}{k-k'} dk = f_1(k',k') , \tag{A.8}$$

$$\lim_{L\to\infty} \int_{-\infty}^{\infty} f_2(k,k') \frac{\cos\{(k-k')L\}}{k-k'} dk = 0 , \tag{A.9}$$

$$\lim_{L\to\infty} \int_{-\infty}^{\infty} f_3(k,k') \frac{\sin\{(k+k')L\}}{k+k'} dk = f_3(-k',k') , \tag{A.10}$$

$$\lim_{L\to\infty} \int_{-\infty}^{\infty} f_4(k,k') \frac{\cos\{(k+k')L\}}{k+k'} dk = 0 . \tag{A.11}$$

In accordance with Eq. (A.8) –Eq. (A.11) for the functions (A.7) in the generalized meaning, we can write

$$\lim_{L\to\infty} \frac{\sin(k-k')L}{k-k'} = \pi\delta(k-k') ,. \quad \lim_{L\to\infty} \frac{\cos(k-k')L}{k-k'} = 0 , \tag{A.12}$$

$$\lim_{L\to\infty} \frac{\sin(k+k')L}{k+k'} = \pi\delta(k+k') , \quad \lim_{L\to\infty} \frac{\cos(k+k')L}{k+k'} = 0 \ . \tag{A.13}$$

Here the factor π appears due to the value of integral $\int_{-\infty}^{\infty} \frac{\sin\{yL\}}{y} dy = \pi$.

Note that the quantities k and k' have the same sign, so that the generalized function $\delta(k+k')$ would be considered as equal to zero ($\delta(k+k') = 0$) since there are no values of k and k' providing the equality $k + k' = 0$. In accordance with the above mentioned, in the limit $L \to \infty$ Eq. (A.1) can be written as

$$\int_{-\infty}^{\infty} \Psi_1(x,k)\Psi_2^*(x,k')\, dx = \pi\ f_1(k,k)\delta(k-k'). \tag{A.14}$$

It is easy to check that if one takes $\Psi_1(x,k) = \Psi_{left}(x,k)$, $\Psi_2(x,k') = \Psi_{left}(x,k')$ or $\Psi_1(x,k) = \Psi_{right}(x,k)$, $\Psi_2(x,k') = \Psi_{right}(x,k')$,then $f_1(k,k) = 2$ (see Eq. (A.3)). Indeed, for the left scattering problem we have

$$a_1 = a_2 = 1,\ d_1 = d_2 = 0 \ \text{ and } \ c_1(k) = c_2^*(k) = t(k),\ b_1(k) = b_2^*(k) = r(k) \tag{A.15}$$

and for the right scattering problem

$$a_1 = a_2 = 0\,,\; d_1 = d_2 = 1 \text{ and } c_1(k) = c_2^*(k) = p(k)\,,\; b_1(k) = b_2^*(k) = s(k)\,. \qquad \text{(A.16)}$$

Inserting Eq. (A.15) or Eq. (A.16) in Eq. (A.3) and taking into account Eq. (A.9) and Eq. (A.10), one can reproduce the equality $f_1(k,k) = 2$.

For the case $\Psi_1(x,k) = \Psi_{left}(x,k)$, $\Psi_2(x,k') = \Psi_{right}(x,k')$ one can write

$$a_1 = 1\,,\; a_2 = 0\,,\; d_1 = 0\,,\; d_2 = 1 \text{ and } c_1(k) = t(k)\,,\; c_2^*(k) = p(k)\,,\; b_1(k) = r(k)\,,\; b_2^*(k) = s(k)\,. \text{(A.7)}$$

In accordance with Eq. (A.3) for this casedue to Eq. (11) we have

$$f_1(k,k) = t(k)p^*(k) + r(k)s^*(k) = 0\,.$$

So, we proved that the wave functions of the left and right scattering problems are orthogonal to each other in Hilbert space. Note that for the case, when $\Psi_1(x,k) = \Psi_{right}(x,k)$, $\Psi_2(x,k') = \Psi_{left}(x,k')$ the equality $f_1(k,k) = 0$ takes place as well.

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