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Matter Wave Evolution for One Dimensional Potential

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Abstract. It is shown that the wave functions ofthe left and right scattering problems can be used as a base for description of a wave process evolution. It is proved that for a same value energy these wave functions are orthogonal to each other. In general form the normalization of the scattering wave functions is done. The well-known result of the transfer matrix is generalized for the case of a complex potential.

Keywords: one dimensional scattering problem, normalization, wave packet

Introduction

In this workwe discuss the wave evolution problem on the base of matter waves propagating in a one-dimensional non-regular media with time independent parameters describing by means of $U(x)$ potential energy. It is known that for matter waves any wave process should take place in accordance with the one-dimensional time dependent Schrödinger equation [2];

$$i\hbar\frac{\partial\Phi(x,t)}{\partial t}=\hat{H}\Phi(x,t),\ \hat{H}=-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+U(x). \tag{1}$$

Espect to this equation the function $\Phi(x,t)$ should satisfy to the condision:

$$\int_{-\infty}^{\infty}\Phi(x,t)\Phi^*(x,t)dx=\int_{-\infty}^{\infty}\Phi_0(x)\Phi_0^*(x)dx=1, \tag{2}$$

where $\Phi_0(x)=\Phi(x,0)$ is a form of a wave perturbation for a time initial moment.

An important class of solutions of Eq.(1) is so-called stationar solutions when the time dependancehas the form of:

$$\Phi(x,t)=\varphi(x,k)\exp\left\{-i\frac{\hbar k^2}{2m}t\right\}, \tag{3}$$

where the function $\varphi(x,k)$ is a solution of an one dimensional Schrödinger stationar equation;

$$\frac{d^2\varphi(x,k)}{dx^2}+\left[k^2-u(x)\right]\varphi(x,k)=0,$$

where $k=\sqrt{2mE}/\hbar$, $u(x)=2mU(x)/\hbar^2$ and E is a total energy. Futher, we will suggest that $u(x)\to 0$ when $x\to\pm\infty$.

The last equation can have two types of solutions corresponding to the finite and infinite motions. For a finite motion (bound states), when an energy takes certain negative values $k^2 = -\chi_n^2$ and a wave function $\varphi(x,k) = \varphi(x, i\chi_n) = \varphi_n(x)$ vanishes for $x \to \pm\infty$ then it can be written:

$$\int_{-\infty}^{\infty} \varphi_n(x)\varphi_{n'}^*(x)dx = \delta_{nn'}, \tag{5}$$

where $\delta_{nn'}$ is Kronecker symbol. Note that a bound state can be considered as a real function accurate to an exponential factor.

For infinite motions the normalization of wave functions in the form of Eq.(2) can not be done. For this case a wave function is normalized to delta-function;

$$\int_{-\infty}^{\infty} \varphi(x,k)\varphi(x,-k')dx = \delta(k-k'). \tag{6}$$

where $\varphi(x,-k)$ is a conjugate function of $\varphi(x,k)$ which is obtained from $\varphi(x,k)$ by changing of a sign of a wave number k to opposite. The conjugate function, which is obtained from $\varphi(x,k)$ by means of non algebraic, is a solution of Schrodinger equation as well [3,4];

$$\frac{d^2\varphi(x,\pm k)}{dx^2} + \left[k^2 - u(x)\right]\varphi(x,\pm k) = 0. \tag{7}$$

For a real potential $u(x)$ the function $\varphi(x,-k)$ can be considered asa complex conjugate of $\varphi(x,k)$.

Any solution of Eq. (4) corresponding to an infinite motion is defined up to two constants which are given in its asymptotic behavior, i.e. an asymptotic behavior defines a solution. So, in general, the asymptotic behavior can be written:

$$\varphi(x,k) = \begin{cases} a\exp\{ikx\} + b(k)\exp\{-ikx\}, & x \to -\infty, \\ c(k)\exp\{ikx\} + d\exp\{-ikx\}, & x \to +\infty, \end{cases} \tag{8}$$

where a, d are given quantities and $b(k), c(k)$ should be found. If $k > 0$ then a, d are amplitudes of converging or incoming waves and $b(k), c(k)$ are amplitudes of deverging or outcoming waves. As it follows from Eq. (8), the function $\varphi(x,-k)$ satisfies to the following condition:

$$\varphi(x,-k) = \begin{cases} a\exp\{-ikx\} + b(-k)\exp\{ikx\}, & x \to -\infty, \\ c(-k)\exp\{-ikx\} + d\exp\{ikx\}, & x \to +\infty. \end{cases} \tag{9}$$

Now for this solution the given quantities a, d are the amplitudes of deverging waves and unkown quantities $b(-k), c(-k)$ are amplitudes of converging waves. In accordance with the above mentioned the functions $\varphi(x,k)$ and $\varphi(x,-k)$ are called the coverging and deverging solutions of stationar wave equation.

Below we consider wave processes constructed on the base of wave functions corresponding to theinfinite motion:

$$\Phi(x,t) = \int_{-\infty}^{\infty} \nu(k)\varphi(x,k)\exp\left\{-i\frac{\hbar k^2}{2m}t\right\}dk, \tag{10}$$

where $\varphi(x,k)$ has an asymptotic behavior Eq.(8). It is easy to check that when $\varphi(x,k)$ is normalized as Eq. (6) and

$$\int_{-\infty}^{\infty} \nu(k)\nu(-k)dk = 1, \tag{11}$$

then $\Phi(x,t)$ satisfies to the condition (2). So, for consideration of a wave process Eq. (10) based of the wave functions of an infinite motion Eq. (8) it is improtant that these functions to be exactly normalized on delta-function. Below we consider a problemhow the wave functions of an infinite can be normalized on delta-function.

2. Normalization of the wave functions of an infinite motion

Let us consider the Wronskian of Eq. (4);

$$W = \left[\varphi_1(x,k),\varphi_2(x,k)\right] = \left[\varphi_1(x,k)\frac{d\varphi_2(x,k)}{dx} - \varphi_2(x,k)\frac{d\varphi_1(x,k)}{dx}\right], \tag{12}$$

where $\varphi_1(x,k),\varphi_2(x,k)$ are independent solutions of Eq. (4) corresponding to the same magnitude of k^2. So, one can choose as independent solutions the converging and diverging solutions Eq. (8), Eq. (9);

$$\varphi_1(x,k) = \varphi(x,k),\ \varphi_2(x,k) = \varphi(x,-k)\,. \tag{13}$$

It is well known that for any two solutions the Wronskian does not depend on x [2];

$$W(x) = const \text{ or } dW(x)/dx = 0\,.$$

The given property of the Wronskian can be presented as well:

$$W(x\to+\infty) - W(x\to-\infty) = 0. \tag{14}$$

From Eq. (12) – Eq. (14) and Eq. (8), Eq. (9) one can get

$$a^2 + d^2 = b(k)b(-k) + c(k)c(-k)\,, \tag{15}$$

which means that the sums of intensities of converging and diverging waves equal to each.

Let us consider the following identity:

$$\varphi_1(x,k)\varphi_2(x,-k') = \frac{1}{k^2-k'^2}\frac{d}{dx}\left[\varphi_1(x,k)\frac{d\varphi_2(x,-k')}{dx} - \varphi_2(x,-k')\frac{d\varphi_1(x,k)}{dx}\right] \quad (16)$$

or

$$\int_{-L}^{L}\varphi_1(x,k)\varphi_2(x,-k')dx = \frac{1}{k^2-k'^2}\left[\varphi_1(x,k)\frac{d\varphi_2(x,-k')}{dx} - \varphi_2(x,-k')\frac{d\varphi_1(x,k)}{dx}\right]\Bigg|_{-L}^{L}. \quad (17)$$

where $\varphi_1(x,k)$ and $\varphi_2(x,-k')$ are arbitrary converging and diverging solutions of Eq. (4) (see Eq. (7)).

Using the asymptotic forms of converging and diverging solutions Eq. (8) and Eq. (9), from Eq. (17) it can be written:

$$\int_{-L}^{L}\varphi_1(x,k)\varphi_2(x,-k')dx = v_1(k,k')\frac{\sin[(k-k')L]}{k-k'} + v_2(k,k')\frac{i\cos[(k-k')L]}{k-k'} +$$
$$+ v_3(k,k')\frac{\sin[(k+k')L]}{k+k'} + v_4(k,k')\frac{i\cos[(k+k')L]}{k+k'}, \quad (18)$$

where

$$v_1(k,k') = b_1(k)b_2(-k') + c_1(k)c_2(-k') + a_1a_2 + d_1d_2, \quad (19)$$

$$v_2(k,k') = b_1(k)b_2(-k') + c_1(k)c_2(-k') - a_1a_2 - d_1d_2, \quad (20)$$

$$v_3(k,k') = a_1\cdot(b_2(-k') + b_1(k)) + d_2\cdot(c_2(-k') + c_1(k)), \quad (21)$$

$$v_4(k,k') = a_2\cdot(b_2(-k') - b_1(k)) + d_2\cdot(c_2(-k') - c_1(k)), \quad (22)$$

where $a_1, d_1, b_1(k), c_1(k)$ and a_2, d_2, $b_2(-k'), c_2(-k')$ are the corresponding amplitudes of the solutions $\varphi_1(x,k)$ and $\varphi_2(x,-k')$.

For very large values of L the left part of the equality (18) contains fast oscillating factors in the following forms:

$$\sin[yL]/y,\ \cos[yL]/y, \quad (23)$$

where $y = k-k'$ or $y = k+k'$.The both functions $\sin[yL]/y$ and $\cos[yL]/y$ always tend to zero when $L\to\infty$ for all values of $y\neq 0$.

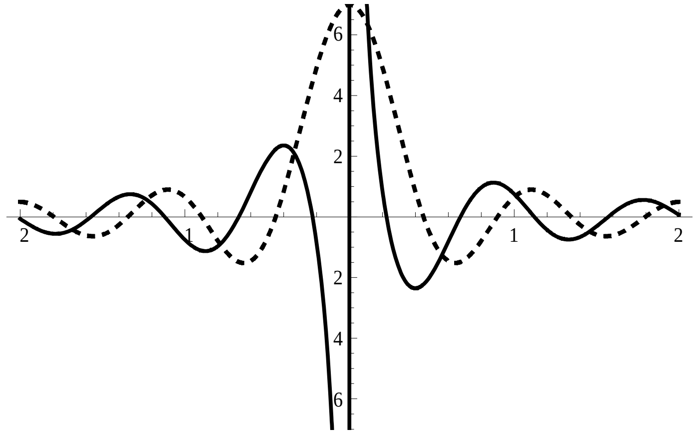

Fig.1. Functions $\sin[yL]/y$ (dashed line) and $\cos[yL]/y$ (continuous line) at $L=7$.

The function $\sin[yL]/y$ is an even function and for the value $y=0$ when $L\to\infty$ it tends to $+\infty$. The function $\cos[yL]/y$ is an odd function, whose value for $y=0$ is uncertain. When $y\to+0$ then $\cos[yL]/y$ tends to $+\infty$ and for the case of $y\to-0$ this function tents to $-\infty$. Note that the functions Eq. (23) as generalized functions,

$$\int_{-\infty}^{\infty}\sin[yL]/y dy=\pi \text{ and } \int_{-\infty}^{\infty}\cos[yL]/y\, dy=0,$$

are (see for example [2]):

$$\sin[yL]/y=\pi\delta(y) \text{ and } \cos[yL]/y=0. \qquad (24)$$

Since $k,k'>0$ then for the case $y=k+k'$ the quantity $y\neq 0$ so $\sin[yL]/y=0$. It means that in Eq. (24) $y=k-k'$ can be considered.

Using Eq. (24), from Eq. (18) it can be written:

$$\int_{-\infty}^{\infty}\varphi_1(x,k)\varphi_2(x,-k')dx=\lim_{L\to\infty}\int_{-L}^{L}\varphi_1(x,k)\varphi_2(x,-k')dx=\pi v_1(k,k)\delta(k-k'). \qquad (25)$$

When $\varphi_1(x,k)=\varphi(x,k)$, $\varphi_2(x,-k')=\varphi(x,-k')$ are chosen, then by using Eq. (15), Eq. (19) from Eq. (25) it can be written as

$$\int_{-\infty}^{\infty}\varphi(x,k)\varphi(x,-k')dx=2\pi(a^2+d^2)\delta(k-k'). \qquad (26)$$

This formula defines a normalization of wave functions of any asymptotic behavior.

As it follows from Eq. (26), for any a and d a solution of Schrodinger equation written as $\psi(x,k)=\varphi(x,k)/\sqrt{2\pi(a^2+d^2)}$ will be normalized to δ function;

$$\psi(x,k)=\frac{1}{\sqrt{2\pi(a^2+d^2)}}\begin{cases} a\exp\{ikx\}+b(k)\exp\{-ikx\}, & x\to-\infty, \\ c(k)\exp\{ikx\}+d\exp\{-ikx\}, & x\to+\infty, \end{cases} \tag{27}$$

$$\int_{-\infty}^{\infty}\psi(x,k)\psi(x,-k')dx=\delta(k-k'). \tag{28}$$

So, we proved that the normalisation constant for an arbitrary solution is presented by means of constants expresing its asymptotic behavior. It means that this constant does not depend on a scattering potential form.

3. The left and right scattering functions

The scattering process corresponds to an infinite motion. The asymptotic behaviors of the wave functions describing the left and right scattering problems can be written from Eq. (8). So, if $a=1,\ d=0$ then

$$\psi(x,k)=\psi_{left}(x,k) \text{ and } b(k)=r(k),\ c(k)=t(k). \tag{29}$$

and when $a=0,\ d=1$ then

$$\psi(x,k)=\psi_{right}(x,k) \text{ and } b(k)=s(k),\ c(k)=p(k). \tag{30}$$

From Eq. (27) - Eq. (30) for the asymptotic behaviors of the normalized wave functions of left and right scattering problems one can write:

$$\psi_{left}(x,k)=\frac{1}{\sqrt{2\pi}}\begin{cases} \exp\{ikx\}+r(k)\exp\{-ikx\}, & x\to-\infty, \\ t(k)\exp\{ikx\}, & x\to+\infty \end{cases} \tag{31}$$

and

$$\psi_{right}(x,k)=\frac{1}{\sqrt{2\pi}}\begin{cases} s(k)\exp\{-ikx\}, & x\to-\infty, \\ \exp\{-ikx\}+p(k)\exp\{ikx\}, & x\to+\infty, \end{cases} \tag{32}$$

where $t(k)$, $r(k)$ and $s(k)$, $p(k)$ are the transmission and reflection amplitudes of the left and right scattering problem, correspondingly. It is important to note that $k>0$ must be considered.

In accordance with Eq. (31), Eq.(32) the conjugate functions for solutions $\psi_{left}(x,k)$ and $\psi_{right}(x,k)$ have to passess asymptitic behaviors in the forms of:

$$\psi_{left}(x,-k)=\frac{1}{\sqrt{2\pi}}\begin{cases} \exp\{-ikx\}+r(-k)\exp\{ikx\}, & x\to-\infty, \\ t(-k)\exp\{-ikx\}, & x\to+\infty \end{cases} \tag{33}$$

and

$$\psi_{right}(x,-k)=\frac{1}{\sqrt{2\pi}}\begin{cases} s(-k)\exp\{ikx\}, & x\to-\infty, \\ \exp\{ikx\}+p(-k)\exp\{-ikx\}, & x\to+\infty. \end{cases} \tag{34}$$

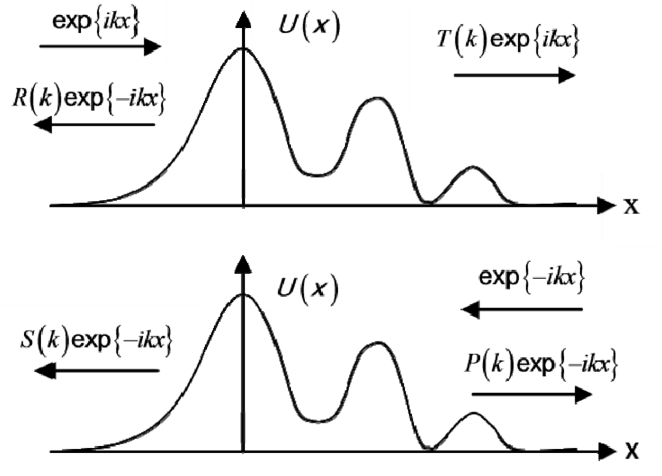

Fig. 2.The left and right scattering problems.

As it was shown in [3, 4], for a real $u(x)$ the replacing of k sign to opposite is equivalent to a complex conjugate action, so that

$$\psi_{left}(x,-k)=\psi^*_{left}(x,k),\ \psi_{right}(x,-k)=\psi^*_{right}(x,k).$$

Below we suggest a very simple and transparency method for derivation of relations acting between the transmission and reflection amplitudes of the left and right scattering problems. Let us consider the Wronskian Eq. (12) written for the following four couples of solutions of Eq. (4) $\psi_{left}(x,k),\ \psi_{right}(x,k), \psi_{left}(x,-k), \psi_{right}(x,-k)$ Eq. (31) - Eq. (34):

$$W_1=\left[\psi_{left}(x,k),\psi_{left}(x,-k)\right], \tag{35}$$

$$W_2=\left[\psi_{right}(x,k),\psi_{right}(x,-k)\right], \tag{36}$$

$$W_3=\left[\psi_{left}(x,k),\psi_{right}(x,-k)\right], \tag{37}$$

$$W_4=\left[\psi_{left}(x,k),\psi_{right}(x,k)\right]. \tag{38}$$

By using Eq. (31) and Eq. (33), it is easy to check that when $W=W_1$ then

$$W(x\to+\infty)=t(k)t(-k)\ ,W(x\to-\infty)=1-r(k)r(-k)$$

and for this case from Eq. (14) one can get:

$$t(k)t(-k)+r(k)r(-k)=1. \tag{39}$$

By using Eq. (32), Eq. (34) for the case of $W=W_2$ it can be found that

$$W(x\to+\infty)=1-p(k)p(-k)\ ,W(x\to-\infty)=s(k)s(-k)$$

and from Eq. (14) one gets:

$$s(k)s(-k)+p(k)p(-k)=1. \tag{40}$$

When $W=W_3$ by using Eq. (31) and Eq. (34) it is found

$$W(x \to +\infty) = t(k)p(-k),\ W(x \to -\infty) = -r(k)s(-k)$$

hence from Eq. (14) one gets:

$$p(-k)t(k) + r(k)s(-k) = 0. \tag{41}$$

For the case of $W = W_4$ by using Eq. (31), Eq. (32) it can be written as

$$W(x \to +\infty) = t(k),\ W(x \to -\infty) = s(k)$$

so that from Eq. (14) one can obtain:

$$t(k) = s(k)\ . \tag{42}$$

Equations (39)-(42) are well known and they lay on a base of the transfer matrix method [1,4]. In particular, the last equation means that the transmission amplitudes of the left and right scattering problems coincide with each other. The basic relations (39)-(42) are usually derived in a framework of group theory [1]. It is obvious that the above suggested appoach is more transparansive.

For any values of a, d the function $\psi(x,k)$ Eq. (27) can be presented by means of a linear combination of $\psi_{left}(x,k)$ and $\psi_{right}(x,k)$ (see Eq. (31));

$$\psi(x,k) = \frac{1}{\sqrt{(a^2 + d^2)}}\left[a\psi_{left}(x,k) + d\psi_{right}(x,k)\right]. \tag{43}$$

Using Eq. (27) and Eq. (31), Eq. (32), from Eq. (43) one gets the well-known connection acting between the amplitudes of diverging and converging waves [1];

$$c(k) = t(k)a + p(k)d\ ,\ b(k) = r(k)a + s(k)d \tag{44}$$

or

$$\begin{pmatrix} c(k) \\ b(k) \end{pmatrix} = \hat{S}\begin{pmatrix} a \\ d \end{pmatrix},\ \hat{S} = \begin{pmatrix} t(k) & p(k) \\ r(k) & s(k) \end{pmatrix},$$

where $\hat{S}$ is called a scattering matrix.

4. The scattering wave functions as a base for description of a wave process evolution

Let us consider a wave process constructed by means of the scattering functions;

$$\Phi(x,t) = \int_0^\infty [\nu_{left}(k)\psi_{left}(x,k) + \nu_{right}(k)\psi_{right}(x,k)]\exp\left\{-i\frac{\hbar k^2}{2m}t\right\}dk\ , \tag{45}$$

where $\nu_{left}(k)$, $\nu_{right}(k)$ define the spectum of a wave process $\Phi(x,t)$ in a base of the functions $\psi_{left}(x,k)$, $\psi_{right}(x,k)$. Now we have to prove that if

$$\int_{-\infty}^{\infty}\left[\nu_{left}(k)\nu_{left}(-k)+\nu_{right}(k)\nu_{right}(-k)\right]dk=1, \tag{46}$$

then for the function $\Phi(x,t)$ Eq. (45) the condition (2) takes place or which is the same as:

$$\int_{-\infty}^{\infty}\Phi(x,0)\Phi^{*}(x,0)dx=\int_{0}^{\infty}\left[\nu_{left}(k)\nu_{left}(-k)+\nu_{right}(k)\nu_{right}(-k)\right]dk=1. \tag{47}$$

So as it follows from Eq. (27) and Eq. (29), Eq. (30) can be written:

$$\int_{-\infty}^{\infty}\psi_{left}(x,k)\psi_{left}(x,-k')dx=\delta(k-k'),\quad \int_{-\infty}^{\infty}\psi_{right}(x,k)\psi_{right}(x,-k')dx=\delta(k-k'). \tag{48}$$

For implementation of Eq. (47), it is nessesary to show that the left and right scattering functions are orthogonal with respect toeach other;

$$\int_{-\infty}^{\infty}\psi_{left}(x,k)\psi_{right}(x,-k')dx=0. \tag{49}$$

It is easy to see that Eq. (49) directry follows from Eq. (25) and Eq. (19). Indeed, for this case when $\varphi_1(x,k)\sim\psi_{left}(x,k),\varphi_2(x,-k)\sim\psi_{right}(x,-k)$ due to the equalities (see Eq. (29))

$$a_1=1,\ d_1=0,\ b_1(k)=r(k),\ c_1(k)=t(k)$$

and (see Eq.(30))

$$a_2=0, d_2=1,\ b_2(k)=s(k),\ c_2(k)=p(k)$$

For the quantity $v_1(k,k)$ one gets:

$$v_1(k,k)=r(k)s(-k)+t(k)p(k).$$

It follows from Eq. (41) that $v_1(k,k)=0$. So, we have proved that the property (49) takes place.

By using Eq. (48), Eq. (49), from Eq. (45) for the spectral $\nu_{left}(k)$, $\nu_{right}(k)$ one can write:

$$v_{left}(k)=\int_{-\infty}^{\infty}\Phi(x,0)\psi_{left}(x,-k)dx,\ v_{right}(k)=\int_{-\infty}^{\infty}\Phi(x,0)\psi_{right}(x,-k)dx. \tag{50}$$

The obtained result shows that the set of the functions $\psi_{left}(x,k),\psi_{right}(x,k)$ is a full orthogonal one, so it allows to conduct a performance of different wave processes with a required asymptotic behavior. So, on the base of the expansion (45) one can consider an evolution of a wave process starting as a solitary wave falling to a potential from its left, the right side or from the both sides. The last case is more interesting one because of the bound states can be considered and obtained as an evaluation result of wave packets.

Conclusion

Thus, we have proved that a system of wave functions of the left and right scattering problems has the completeness property for description of the matter wave evolution. For any form of an infinite motion, the normalization of the wave function is done.

The generalization of the well-known formulas of the transfer matrix method is done [1]. It is shown that for a case of a complex potential the action of the complex conjugation for the scattering amplitudes is changed to the action of alteration of the wave number sign.

The approach of quantum wave description, as it is presented in the subject work, can be permeated on linear waves with different species as well. In particular, it can be electromagnetic waves, hydro waves, the waves in the solid states, and etc. Application of the results deriving from this work is notably wide and it is able to find its utilization in different areas of natural sciences in the nearest future.

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