The normalization and the boundary condition of a particle wave function moving in a field of an arbitrary one-dimensional potential

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Abstract: The normalization problem of a wave function for an arbitrary one-dimensional field is considered. It is shown, that for an infinite motion type the magnitude of the normalization constant does not depend on the form of a scattering potential and it is determined by the boundary conditions imposed on the character of the investigated motion. The general formula for the normalization constant as a function of amplitudes of the waves converging to the potential is derived.

Keyword: Normalization problem, wave function, one-dimensional motion, arbitrary potential

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I. Introduction

It is known that the normalization condition of the wave function is one of the basic concepts of quantum mechanics. This condition is important to describe the probabilistic nature of the physical quantities characterizing the various properties of microscopic systems [1]. Thus, depending on the motion characteristics, i.e. whether or not the motion takes place in a finite or an infinite area of space, the wave function must be normalized to unity or δ - function, respectively. The question is how the normalization constant depends on the asymptotic behavior depositing on a wave function behavior.

In this paper we analyze the normalization problem of the wave function for an infinite motion in the case of one-dimensional Schrödinger equation:

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

\[ k = \frac{\sqrt{2mE}}{\hbar}, \quad u(x) = \frac{2mU(x)}{\hbar^2}, \]

\( E \) and \( U(x) \) are the total and potential energy, respectively.

The limitation for the review given below is the form of the potential energy. In accordance with Fig. 1 the magnitudes of the potential at the infinites tend to zero when \( |x| \to \infty \). It also seems that when \( k^2 > 0 \) the motion occurs in infinite area, i.e. in whole space, and when \( k^2 < 0 \) the motion character is finite.

To specify the formulation of the problem, as a rule, the wave function \( \Psi(x) \) is written as function \( \Psi_k(x) \) depending on the parameter \( k \), the asymptotic behavior of which in its most general form is written as follows:

\[ \Psi_k(x) = \begin{cases} A_1 \exp\{ikx\} + B_1 \exp\{-ikx\}, & x \to -\infty, \\ A_2 \exp\{ikx\} + B_2 \exp\{-ikx\}, & x \to +\infty. \]  

On conditions that \( k > 0 \) the quantities \( A_1, B_1 \) will be the amplitudes of waves converging to the potential of waves and the quantities \( A_2, B_2 \) will be the amplitudes of outgoing waves. It is clear that when \( k < 0 \), \( A_1, B_2 \) and \( A_2, B_1 \) will be amplitudes of diverging and converging waves, respectively.

Formulation of the problem can be concretized, if any two of the four variables \( A_1, B_1, A_2, B_2 \) are treated as initially specified. In other words, the wave equation determines the wave function only up to two arbitrary constants. It is clear that the choice of a pair from the four constants can be carried out in various ways.
Thus, as the originally specified amplitudes the following pairs may be considered: \((A_1, B_1), (A_2, B_2), (A_3, B_3), (A_4, B_4)\). For the above written order of the pairs the required ones will be \((A_3, B_3), (A_4, B_4), (A_2, B_2), (A_1, B_1)\) respectively. It’s clear, that under the linearity of the Schrodinger equation, there is always a linear relationship between the given and unknown quantities.

![Potential region](image)

**Fig. 1** Form of the potential, and the range of values of energy for finite and infinite motions.

This work is devoted to finding a link between the constant of normalization of the wave function of infinite motion and the amplitudes that determine the asymptotic behavior of the wave function of the converging and diverging waves.

### II. Method of converging waves

Consider a pair of functions \(a_k(x), b_k(x)\), which satisfies the following system of linear differential equations [2-4]:

\[
\frac{da_k(x)}{dx} = \frac{i u(x)}{2k} a_k(x) - \frac{i u(x)}{2k} b_k(x) \exp\{-i2kx\}, \tag{4}
\]

\[
\frac{db_k(x)}{dx} = \frac{i u(x)}{2k} b_k(x) + \frac{i u(x)}{2k} a_k(x) \exp\{i2kx\}. \tag{5}
\]

Let's compose the following function on the basis of functions \(a_k(x), b_k(x)\):

\[
\Psi_k(x) = a_k(x) \exp\{ikx\} + b_k(x) \exp\{-ikx\}. \tag{6}
\]

Using equations (4), (5) it is easy to derive that the function satisfies the wave equation (1), and regardless of the type of potential energy \(u(x)\) derivative of the wave function \(\Psi_k(x)\), written by use of \(a_k(x), b_k(x)\), has the form:

\[
\frac{d\Psi_k(x)}{dx} = ik [a_k(x) \exp\{ikx\} - b_k(x) \exp\{-ikx\}]. \tag{7}
\]

To obtain the wave function \(\Psi_k(x)\) (6) the system of equations (4), (5) can be solved. Depending on the asymptotic behavior put on the wave function, i.e. the choice in the asymptotic form (3) a pair of amplitudes which are initially considered as given quantity, the system of equations (4), (5) have to be considered for a given boundary condition or for a given initial conditions. Depending on \(t\), thus, if in the asymptotic condition for the wave function \(\Psi_k(x)\) the amplitudes on one side of potential are given, then the system of equations for the functions (4), (5) will be solved with given initial condition. And if for function \(\Psi_k(x)\) the amplitudes of the waves \(a_k(x), b_k(x)\) on both sides of potential are given, then the system (4), (5) should be solved as a boundary value problem. Both the initial and the boundary value problems can be formulated in two ways.

If the initial condition for the system (4), (5) is given for \(x \to -\infty\), i.e.

\[
a_k(x \to -\infty) = A_k, \quad b_k(x \to -\infty) = B_k, \tag{8}
\]

where \(A_k \) and \(B_k \) are constants, then the solution of (6) will determine the wave function with asymptotic behavior
The boundary value problem asymmetric with respect to (14) to the potential waves are given. The solution \( \Psi_k(x) \) is called a convergent solution of the wave equation. The boundary value problem asymmetric with respect to (14) is also interesting, where the value of the function \( a_k(x) \) is given already on the right side of the potential, and for the function \( b_k(x) \) it’s given on the left side;

\[
\Psi_k(x) = a_k(x \to +\infty) = A_2^+ \quad \text{and} \quad b_k(x \to -\infty) = B_1^- ,
\]

where \( A_2^+ \) and \( B_1^- \) are predetermined constants. Under the condition (16) functions \( a_k(x) \), \( b_k(x) \) determine the solution (6), for which the amplitudes of waves diverging from the potential will be given. In this connection, such a solution is called divergent;

\[
\Psi_k(x) \equiv \Psi_k^+(x) = \begin{cases} A_1^+ \exp \{ikx\} + B_1^+ \exp \{-ikx\}, & x \to -\infty, \\ A_2^+ \exp \{ikx\} + B_1^- \exp \{-ikx\}, & x \to +\infty, \end{cases}
\]

As in the case of convergent solutions (15), for the solution (17) the amplitudes of waves for both positive and negative large values of \( x \) are given, but in this case, it will be divergent waves from the potential. Therefore, divergent solutions, we will mark with “+” to distinguish it thereby from a convergent solution, which was marked with “-+” (see (18)).
The relationship between the amplitudes of converging and diverging waves realizes by so-called scattering matrix $\hat{S}(k)$ [3-7]. Regardless of the form of scattering potential $u(x)$, the relationship between the amplitudes of the unknown and the given waves has the form:

$$
\begin{pmatrix}
A_2(k) \\
B_2(k)
\end{pmatrix} = \hat{S}(k) \begin{pmatrix}
A_1^* \\
B_1^*
\end{pmatrix} = \begin{pmatrix}
1/\alpha(-k) & \beta(k)/\alpha(-k) \\
-\beta(-k)/\alpha(-k) & 1/\alpha(-k)
\end{pmatrix} \begin{pmatrix}
A_1^* \\
B_1^*
\end{pmatrix}.
$$

The relationship between unknown and given amplitudes of divergent solution (19) can be conveniently written by means of the matrix $\hat{S}^{-1}(k)$, i.e. by means of the inverse matrix of the scattering matrix:

$$
\begin{pmatrix}
A_1(k) \\
B_1(k)
\end{pmatrix} = \hat{S}^{-1}(k) \begin{pmatrix}
A_2 \\
B_2
\end{pmatrix} = \begin{pmatrix}
1/\alpha(k) & -\beta(k)/\alpha(k) \\
\beta(-k)/\alpha(k) & 1/\alpha(k)
\end{pmatrix} \begin{pmatrix}
A_2 \\
B_2
\end{pmatrix}.
$$

It is important to note that the forms of the transfer matrix $\hat{T}$ (11) and the scattering matrix $\hat{S}$ (18) remain valid even when the potential and the total energy $u(x)$ and $k^2$ are considered as complex quantities. For the case of real function $u(x)$, as well as when $k^2$ is real, the replacement of the sign of $k$ on opposite $-k$ in the matrix (11) is equivalent to the action of complex conjugation [6] (see also [4]):

$$
\alpha(-k) = \alpha^*(k), \quad \beta(-k) = \beta^*(k),
$$

where “*” means complex conjugation.

### III. The initial and boundary value problems for finding a solution to the wave equation

As noted above, the wave function of one-dimensional motion, depending on the formulation of the problem, can be defined as the initial value problem or as a boundary value problem for a system of linear differential equations. For the first case the amplitudes of the waves on one side of the potential considered known, in the second case the amplitudes of the waves on either side of the potential considered known.

In general, the various formulations of the problem lead to a linearly independent of each other's solutions of the wave equation. However, in a certain relation between the amplitudes of the waves given with initial and boundary conditions, different formulations of the problem will lead to the same solution. For example, if the values of the wave amplitudes for the left and right initial value problems connected with a transfer matrix, the corresponding wave functions will be the same. In the case of boundary value problems (15), (17), when the wave amplitudes for the converging and diverging solutions are connected through the $\hat{S}$-matrix (18):

$$
\begin{pmatrix}
A_2 \\
B_1
\end{pmatrix} = \begin{pmatrix}
1/\alpha(-k) & \beta(k)/\alpha(-k) \\
-\beta(-k)/\alpha(-k) & 1/\alpha(-k)
\end{pmatrix} \begin{pmatrix}
A_1 \\
B_2
\end{pmatrix},
$$

the converging and diverging solutions will coincide:

$$
\Psi_k^+(x) = \Psi_k^-(x).
$$

Let $\Psi_k^+(x)$ be a convergent solution of the wave equation (1). For example, the wave functions corresponding to the left and right scattering problems are convergent solutions:

$$
\Psi_k^{left}(x) = \begin{cases}
\exp{ikx} + r(k)\exp{-ikx}, & x \to -\infty, \\
\exp{ikx}, & x \to +\infty
\end{cases}
$$

and

$$
\Psi_k^{right}(x) = \begin{cases}
s(k)\exp{-ikx}, & x \to -\infty, \\
\exp{-ikx} + p(k)\exp{ikx}, & x \to +\infty
\end{cases}
$$

where the quantities $r(k), t(k)$ and $p(k), s(k)$ will be the amplitudes of the reflection and transmission waves, correspondingly when the primary wave falls on the barrier on the left and when it falls on the barrier on the right. It is easy to see that in the case of the left scattering problem the amplitudes of convergent (given) and divergent (required) waves equal, respectively,

$$
A_1^+ = 1, \quad B_2^- = 0 \quad \text{and} \quad A_2 = t(k), \quad B_1 = r(k).
$$

In the case of right scattering problem

$$
A_1^- = 0, \quad B_2^+ = 1 \quad \text{and} \quad A_2 = p(k), \quad B_1 = s(k).
$$
Consider the function $\Psi^+_{-k}(x)$ derived from the function $\Psi^+_{k}(x)$ of the convergent solution (15) by non-algebraic action, but namely by replacement of $k$ on $-k$:

$$\Psi^+_{-k}(x) = a_{-k}(x) \exp \{-ikx\} + b_{-k}(x) \exp \{ikx\},$$

(27)

where the functions $a_{-k}(x), b_{-k}(x)$ are obtained from the functions $a_{k}(x), b_{k}(x)$ with replacement $k$ on $-k$. Following the paper [3], we can show that the function $\Psi^+_{-k}(x)$ appears to be a divergent solution of the wave equation, i.e.

$$\Psi^+_{-k}(x) = \Psi^+_{k}(x),$$

(28)

and for the amplitudes of outgoing waves from the potential we get

$$A_2 = B_2^* \text{ and } B_1 = A_1^*,$$

(29)

where $A_1^*, B_1^*$ are the given amplitudes for the converging solution $\Psi^+_{k}(x)$ (see (15)).

It is reasonable to name the functions $\Psi^+_{k}(x)$ and $\Psi^+_{-k}(x)$, connected by the relation (28), converging and diverging solutions conjugated to each other.

Thus, in the case of real potential, when the wave amplitudes $A_1^*, B_1^*$ can take only real values (for example, (23), (24)), the effect of replacing the sign of $k$ on the opposite sign is equivalent to the action of complex conjugation, i.e. $\Psi_{-k}(x) = \Psi^+_{k}(x)$.

IV. The normalization of the wave function of infinite motion

Next, we investigate the following integral

$$\int_{-\infty}^{\infty} \Psi^+_{k}(x)\Psi^+_{k'}(x) dx = \int_{-\infty}^{\infty} \Psi_{k}(x)\Psi_{k'}(x) dx,$$

(30)

which contains the product of conjugate solutions, where considered the notation $\Psi^+_{k}(x) = \Psi_{k}(x)$ for convergent solutions, and the divergent solution is represented in the form $\Psi^+_{-k}(x) = \Psi_{-k}(x)$ in accordance with (28). It is clear that in the case of the real potential this integral is transformed into the corresponding integral, which determines the normalization of the wave function:

$$\int_{-\infty}^{\infty} \Psi_{k}(x)\Psi_{-k'}(x) dx = \int_{-\infty}^{\infty} \Psi^+_{k}(x)\Psi^+_{-k'}(x) dx.$$

In order to study the integral (30), we’ll use the known identity [1]

$$\int_{-L}^{L} \Psi^+_{k}(x)\Psi^+_{k'}(x) dx = \frac{1}{k^{2} - k'^{2}} \left[ \Psi^+_{k'}(x) \frac{d\Psi^+_{k}(x)}{dx} - \Psi^+_{k}(x) \frac{d\Psi^+_{k'}(x)}{dx} \right]_{-L},$$

(31)

According to (28), (29), the asymptotic behavior of the solution $\Psi^+_{k}(x)$ has the form

$$\Psi^+_{k}(x) = \left\{ \begin{array}{ll}
A_1^* \exp \{-ik'x\} + B_1(-k') \exp \{ik'x\}, & x \to -\infty, \\
A_2(-k') \exp \{-ik'x\} + B_2^* \exp \{ik'x\}, & x \to +\infty.
\end{array} \right.$$  

(32)

Using (15) and (32), after simple calculations, considering the large values of $L$, we can write the following for (31):

$$\int_{-L}^{L} \Psi^+_{k}(x)\Psi^+_{k'}(x) dx = f_1(k,k') \frac{\sin \{(k-k')L\}}{k-k'} \frac{i\cos \{(k-k')L\}}{k-k'} + f_2(k,k') \frac{\sin \{(k+k')L\}}{k+k'} \frac{i\cos \{(k+k')L\}}{k+k'},$$

(33)

where

$$f_1(k,k') = A_2(-k') A_2(k) + B_1(-k') B_1(k) + A_1^* A_1^* + B_2^* B_2^*,$$

$$f_2(k,k') = A_2(-k') A_2(k) + B_1(-k') B_1(k) - A_1^* A_1^* - B_2^* B_2^*.$$  

(34)
\[ f_3(k, k') = A_2(-k')B_2^+ + B_1(-k')A_1^+ + A_1^+B_1(k) + B_1^+A_2(k), \]  
\[ f_4(k, k') = A_2(-k')B_2^+ + B_1(-k')A_1^+ - A_1^+B_1(k) - B_1^+A_2(k). \]  
When the quantities \( k \) and \( k' \) are treated as real values, then for very large values of \( L \) the expression (33) includes fast oscillating factors of the following behavior:

\[ \frac{\sin\{yL\}}{y}, \quad \frac{\cos\{yL\}}{y}, \]  

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

Definite meaning can be given to the functions (38) in the class of generalized functions. To do this, as you know, it is necessary to consider the values of nonintrinsic integrals in condition of \( L \to \infty \), containing in addition to the functions (38) some smooth functions as integrands. Thus, considering \( dy = dk \) as the difference, we can write

\[ \lim_{L \to \infty} \int_{-\infty}^{\infty} f_1(k, k') \frac{\sin\{(k - k')L\}}{k - k'} dk = f_1(k', k'), \]  
\[ \lim_{L \to \infty} \int_{-\infty}^{\infty} f_2(k, k') \frac{\cos\{(k - k')L\}}{k - k'} dk = 0, \]
\[ \lim_{L \to \infty} \int_{-\infty}^{\infty} f_3(k, k') \frac{\sin\{(k + k')L\}}{k + k'} dk = f_3(-k', k'), \]
\[ \lim_{L \to \infty} \int_{-\infty}^{\infty} f_4(k, k') \frac{\cos\{(k + k')L\}}{k + k'} dk = 0. \]

In accordance with (39) - (42) for the functions (38) in the generalized meaning, we can write

\[ \lim_{L \to \infty} \frac{\sin(k - k')L}{k - k'} = \pi \delta(k - k'), \quad \lim_{L \to \infty} \frac{\cos(k - k')L}{k - k'} = 0, \]
\[ \lim_{L \to \infty} \frac{\sin(k + k')L}{k + k'} = \pi \delta(k + k'), \quad \lim_{L \to \infty} \frac{\cos(k + k')L}{k + k'} = 0. \]

where the factor \( \pi \) is depended on the value of the integral \( \int_{-\infty}^{\infty} \sin yL/ y \quad dy = \pi \).

Note, that it makes sense to consider \( k \) and \( k' \) as variables having the same sign. Because of this, function \( \delta(k + k') \) should also be considered to be zero (\( \delta(k + k') = 0 \)), since for any values \( k \) and \( k' \) the equality \( k + k' = 0 \) cannot be performed. According to our observation, and (43), (44) in the limit \( L \to \infty \) we can write the following for equation (38):

\[ \int_{-\infty}^{\infty} \Psi_{k}^+(x)\Psi_{k'}(x) dx = \pi f_1(k, k)\delta(k - k'). \]

Considering \( k = k' \) and using the properties of the scattering matrix elements (12), we can write \( f_1(k, k) = 2(A_1^+ A_1^+ + B_2^+ B_2^+) \) for (34) and therefore we have for the conjugated solutions \( \Psi_{k'}^+(x), \Psi_{k'}(x) \)

\[ \int_{-\infty}^{\infty} \Psi_{k}^+(x)\Psi_{k'}^+(x) dx = 2\pi(A_1^+ A_1^+ + B_2^+ B_2^+) \delta(k - k'). \]

It is easy to see that the integral that determines the normalization of the wave function is independent of the form of the scattering potential and is determined by the sum of the intensities of the waves converging to the potential.
V. Conclusion

So, the wave function of a continuous spectrum normalized to the \(\delta\)-function up to a certain factor. According to (46), any wave function \(\Psi_k(x)\) can be normalized to \(\delta\)-function with the help of a suitably chosen factor:

\[
\int_{-\infty}^{\infty} \varphi_k(x)\varphi_{-k'}(x)\,dx = \delta(k - k'), \quad \varphi_k(x) = \frac{1}{\sqrt{2\pi}} \frac{\Psi_k(x)}{\sqrt{A^+_1 A^+_2 + B^+_2 B^+_2}}.
\] (47)

Note that \(A^+_1, B^+_2\) are given for the solution \(\Psi_k(x)\), according to the boundary condition for a convergent solution.

It is interesting to apply the result (47) for a specific type of infinite motion, namely, when the boundary condition corresponds to the left or to the right scattering problem. According to (25), (26) \(A^+_1 = 1\) and \(B^+_2 = 0\) for the left scattering problem, and for the right scattering problem - \(A^+_1 = 0\), \(B^+_2 = 1\). Using (46) it’s easy to see that for both problems the quantity \(f_1(k, k) = 2\) and therefore:

\[
\int_{-\infty}^{\infty} \Psi_{-k'}^l(x)\Psi_k^l(x)\,dx = \int_{-\infty}^{\infty} \Psi_{-k'}^r(x)\Psi_k^r(x)\,dx = 2\pi\delta(k - k').
\] (48)

In conclusion we note that proven formula (47) holds in the general case, when the potential energy is considered as a complex function of the coordinate \(x\). This fact greatly expands the scope of the above derived result. In particular, it may be useful for the inverse scattering problem, when the presence in the environment of drains or sources of the particles is modeled by a some kind of optical potential.

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