New about the wave function, “Einstein’s boxes” and scattering a particle on a one-dimensional δ-potential

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Abstract.
The connection between the problem of scattering a particle on a one-dimensional δ-potential with the “Einstein’s boxes” thought experiment is shown. In both cases, the validity of the superposition principle is limited by Einstein’s ‘separation principle’. It is also shown that the generally accepted point of view, according to which “To know the quantum mechanical state of a system implies, in general, only statistical restrictions on the results of measurements”, is fundamentally wrong. First, even the square of the modulus of the wave function imposes more than just statistical restrictions. Second, the phase of the wave function also has a physical meaning – it sets the field of pulses of the ensemble. That is, quantum mechanics not only does not prohibit the simultaneous measurement of the coordinate and momentum of a particle, but also predicts the value of the momentum at that spatial point where the particle will (accidentally) be detected.

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1. Instead of Introduction

1.1. Tunneling time problem and “Einstein’s Boxes”

At present, in the question of describing the scattering of a quantum particle on a one-dimensional δ-potential barrier, a rather contradictory situation has developed. On the one hand, the modern quantum mechanical model (SQM) of this process [1] has been developed at a rigorous mathematical level, in full compliance with the principles of quantum mechanics and, it would seem, should provide an exhaustive explanation of all its physical properties. On the other hand, this process remains a mystery for researchers (see, for example, [2, 3]), since all attempts to investigate its temporal aspects on the basis of SQM have not been crowned with success. The so-called tunneling time problem (TTP), which arises for any one-dimensional short-range potential barrier, turned out to be so confused that not only is there still no generally accepted definition of the tunneling time, but even the reason why it cannot be solved remains unclear.
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Note that the SQM itself has never been questioned. But, as will be shown below, the reason lies precisely in it, since this model is contradictory (and this applies to the model for any other one-dimensional short-range potential barrier). To reveal the essence of this contradiction, we begin with one of the key provisions of the SQM, which describes the process with one-sided incidence of a particle onto a barrier, according to which all scattering states in this problem are asymptotically free as $t \to \mp\infty$. This means that in these two limiting cases the particle does not interact with the barrier, and the region of its localization consists of two disjoint spatial intervals separated by a barrier region in which the probability of finding the particle is strictly zero. For example, in the case of the $\delta$-potential, “given” at the point $x = 0$, two disjoint intervals are the intervals $(-\infty, 0)$ and $(0, \infty)$, separated by a point $x = 0$.

But the same situation arises in “Einstein’s Boxes” thought experiment, which Einstein used against the orthodox doctrine of the completeness of quantum mechanics (see [4, 5, 6, 7, 8, 9] and also [10, 11]). In the scattering problem, division into two “boxes” occurs in the scattering process at $t \to \mp\infty$, and their role is played by the intervals $(-\infty, 0)$ and $(0, \infty)$. In this regard, the search for the cause will begin with an analysis of the standard quantum-mechanical description of this experiment (although in its original version it was about a ball, we will consider the version with a particle).

1.2. “Einstein’s boxes”: separation principle versus superposition principle

According to Einstein, the standard (orthodox) quantum mechanical description of this experiment contains a contradiction, the essence of which he formulated as follows (quoted from [6, 7]): “the paradox forces us to relinquish one of the following two assertions:

1. the description by means of the $\psi$-function is complete,
2. the real states of spatially separated objects are independent of each other.

On the other hand, it is possible to adhere to (2) if one regards the $\psi$-function as the description of a (statistical) ensemble of systems (and therefore relinquishes (1)). However, this view blasts the framework of the ‘orthodox quantum theory’.”

But, in our opinion, this formulation inaccurately reflects the essence of the contradiction that arises when describing this experiment within the orthodox approach (following the [6], statement (2) we will consider as the “separation principle”). First, assertion (2) contains a sufficient, but not a necessary condition for incompleteness of quantum mechanics: assertion (1) really contradicts assertion (2); but $\psi$-function gives an incomplete description of the particle dynamics in the case of a single box too (it would be strange if in an experiment with two boxes the wave function gave an incomplete description, and in an experiment with one box it did a complete one). And here it should be recalled (see [8]) that Einstein himself did not always use the separation principle to prove the incompleteness of quantum mechanics.

Second, this formulation is based on the assumption (see also [12]) that the transition from the orthodox interpretation of the wave function to the statistical
interpretation (SI) is quite sufficient to reconcile quantum mechanics with the separation principle. However, it is not. What actually contradicts in the traditional quantum-mechanical description of an experiment with two boxes isolated from each other is its provision that the superposition of two pure states of a particle localized in the independent boxes should also be considered as a pure state. And what is important, this contradicts not only position (2), which Einstein formulated, but also the definition of mixed states, which is inherent in quantum mechanics itself.

Let’s dwell on this issue in more detail. Let \( H \) be the Hilbert space associated with this thought experiment. And let \( \psi_1 \) and \( \psi_2 \) be two unit vectors from \( H \), which describe the states of the particle localized in the first and second boxes, respectively. Consider the superposition

\[
\psi = \alpha_1 e^{i\lambda_1} \psi_1 + \alpha_2 e^{i\lambda_2} \psi_2,
\]

(1)

where \( \lambda_1 \) and \( \lambda_2 \) are arbitrary (real) phases, and real parameters \( \alpha_1 \) and \( \alpha_2 \) satisfy the condition \( \alpha_1^2 + \alpha_2^2 = 1 \). The question arises: “Is this a pure state or a mixed state?”

According to orthodox quantum mechanics, all state vectors from \( H \) and their superposition describe pure states, and any observable \( \hat{O} \) corresponds to a self-adjoint operator \( \hat{O} \), whose domain of definition is everywhere dense in \( H \). Therefore, on the one hand, the \( \psi \) state should be treated as pure, and the average \( \langle \psi | \hat{O} | \psi \rangle \) should depend on all four parameters, including the \( \lambda_1 \) phases and \( \lambda_2 \).

On the other hand, if we take into account Exp. (1) for \( \psi \) and the fact that the states \( \psi_1 \) and \( \psi_2 \) are localized in two disjoint spatial regions (the formulation of a thought experiment assumes that they are separated infinitely deep potential well) and, thus, \( \langle \psi_1 | \hat{O} | \psi_2 \rangle = 0 \), then

\[
\langle \psi | \hat{O} | \psi \rangle = \alpha_1^2 \cdot \langle \psi_1 | \hat{O} | \psi_1 \rangle + \alpha_2^2 \cdot \langle \psi_2 | \hat{O} | \psi_2 \rangle.
\]

(2)

But, according to quantum mechanics, such expansions are typical of mixed states, so the superposition (1) cannot be considered a pure state (the fact that \( \langle \psi | \hat{O} | \psi \rangle \) does not depend on the phases \( \lambda_1 \) and \( \lambda_2 \) is also one of the hallmarks of a mixed state). Thus, in order to reconcile the quantum-mechanical description of this thought experiment with the definition of mixed states and with the separation principle, it is necessary to revise the existing position that all vectors from \( H \) describe pure states; in other words, it is necessary to revise the existing formulation of the principle of superposition in relation to the “Einstein’s boxes”.

1.3. The transition from a pure state into a mixed state in a closed system

However, having settled the contradiction that appears in the standard description of the state of a particle in two boxes, we arrive at something else. The fact is that in this experiment the particle is first located in one box, and only then this box, with the help of an absolutely impenetrable partition, is divided into two boxes independent of each other. This means that a mixed state in this experiment arises only at the final stage, and at the initial moment of time, when there is only one box, the particle is in
a pure state, since Einstein assumed that the state of the particle in the experiment is described by the \( \psi \)-function. Thus, in the course of this experiment, the initially pure state of the particle is transformed into a mixed one. But the fact is that the transition from a pure state to a mixed one, according to orthodox quantum mechanics, is possible only in open systems, thanks to the decoherence process, which is described using a reduced density matrix.

At first glance, in the case of Einstein’s Boxes, this contradiction is easily resolved. First, although Einstein assumed that the state of a particle is described by a \( \psi \)-function, an exact quantum-mechanical analysis of the dynamics of a particle, as a closed system, is impossible within the framework of his purely speculative setting of this problem. Secondly, dividing the original box into two using an ideal impenetrable partition involves the intervention of an external agent. But this means that in this experiment the particle cannot be considered a closed system; the process of decoherence occurs precisely due to this external interference.

Thus, the thought experiment itself cannot be viewed as a serious challenge for the traditional scenario of the system’s transition from a pure state to a mixed state (in fact, this is another reason why Einstein’s criticism was not properly received). However, such a scenario does not work in the case of a particle scattering on a one-dimensional \( \delta \)-potential barrier – an analogue of the Einstein Boxes. At all stages of this process, the particle is a closed system, the state of which is described by the wave function. Thus, the SQM – the existing model of this process – must be revised, since the appearance of a mixed state when \( t \to \infty \) should inevitably lead, in the Schrodinger formalism, to a restriction of the superposition principle in the corresponding Hilbert state space and, consequently, to new physics of this process.

Note that the concept of a mixed vector state is itself unusual in Schrodinger’s formalism. Therefore, before to proceed to a revision of the SQM, we must first understand what restrictions the wave function imposes on the physical properties of this unusual quantum state and how these restrictions differ from those imposed on a pure state and a mixed state determined with the density operator. In doing so, we must proceed from the doctrine of the incompleteness of quantum mechanics, according to which quantum mechanics is the theory of quantum statistical ensembles. In this regard, we will adhere to the statistical interpretation (SI) [12], which, in our opinion, most accurately reflects the essence of quantum mechanics.

In principle, we could resolve this question during the revision of the SQM. However, we are forced to highlight it separately, since at present quantum mechanics gives a false idea of these limitations even in the case of an ordinary, pure quantum state. For example, in the very first phrase of his book [13], John Bell writes “To know the quantum mechanical state of a system implies, in general, only statistical restrictions on the results of measurements”. This idea, based on the Born interpretation of the wave function, is so ingrained in modern quantum mechanics that it is considered an immutable fact. It is this idea that underlies long debate on the foundations of quantum mechanics.
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Against this background, the Bohm approach stands out. In the works [14, 15] David Bohm showed that if we introduce into quantum mechanics an additional postulate on the existence of single-particle trajectories, then the phase of the wave function determines the particle momentum, and its modulus determines not only statistical restrictions but also the quantum-mechanical potential. As a consequence, in this approach, the quantum mechanical state implies not only statistical restrictions on the measurement results.

It is generally accepted that the wave function acquires these properties only due to the postulate about trajectories. And since this postulate does not fit into the framework of quantum mechanics, Bohm’s finds were not taken, anyhow, into account in other interpretations of quantum mechanics, including SR. At the same time, as will be shown in the next section, these finds, with corresponding corrections, also arise in SI, where there is no postulate about trajectories.

2. Physical meaning of the modulus and phase of the wave function

2.1. Pure state

Let us begin with a pure state

$$\psi(x, t) = \sqrt{w(x, t)} e^{i\phi(x, t)}, \quad (3)$$

where \(w(x, t)\) and \(\phi(x, t)\) are real functions; \(\int_{-\infty}^{\infty} w(x, t) dx = 1; w(x, t) \geq 0\). According to Max Born, \(w(x, t) = |\psi(x, t)|^2\) is the probability density, and in SI (see [12]) it is a function describing the distribution of particles along the coordinate \(x\) at time \(t\) in the corresponding quantum ensemble. As for the phase \(\phi(x, t)\), nothing is said about its physical meaning in SI. To find it out, we write the average value of the momentum operator \(\hat{p} = -i\hbar \frac{d}{dx}\) in the form

$$\langle p \rangle = \int_{-\infty}^{\infty} \psi^*(x, t) \hat{p} \psi(x, t) dx = \int_{-\infty}^{\infty} p(x, t) w(x, t) dx, \quad (4)$$

where

$$p(x, t) = \frac{\text{Re} (\psi^*(x, t) \hat{p} \psi(x, t))}{w(x, t)} = \frac{\hbar}{w(x, t)} \text{Im} (\psi^*(x, t) \psi_x(x, t)) = \hbar \phi_x(x, t) \quad (5)$$

for any function \(f(x, t)\), hereinafter, \(f_x(x, t) \equiv \partial f(x, t)/\partial x\) and \(f_{xx}(x, t) \equiv \partial^2 f(x, t)/\partial x^2\). Thus, not only the function \(w(x, t)\) – the square of the modulus of the wave function \(\psi(x, t)\) – which we will call below the ‘probability field’, has a physical meaning, but also its phase \(\phi(x, t)\), which defines the field of pulses \(p(x, t)\); both fields characterize the physical properties of the quantum ensemble.

Note that the definition of the impulse variable in terms of the phase of the wave function, similar to the definition (5), also appears in Bohm quantum mechanics [14]. But in [14] the coordinate \(x\) depends on \(t\), and the momentum is defined as the particle momentum on a trajectory \(x(t)\). In our approach, the function \(p(x, t)\) depends on two independent variables \(x\) and \(t\), and it is introduced on the basis of a standard formula in
quantum mechanics for calculating the average momentum over an ensemble of particles (see the first equality in Section (4)).

For a quantum ensemble, in addition to the momentum field \( p(x, t) \), the kinetic energy field \( K(x, t) \) can be introduced. For this, we write the average value of the kinetic energy operator \( \hat{K} = \hat{p}^2 / 2m \) in the form
\[
\langle K \rangle = \frac{1}{2m} \int_{-\infty}^{\infty} \psi^*(x, t) \hat{p}^2 \psi(x, t) dx \equiv \int_{-\infty}^{\infty} K(x, t) w(x, t) dx,
\]
where
\[
K(x, t) = \frac{1}{2m} [p(x, t)]^2 - \frac{\hbar^2}{4m} \left[ \frac{w_{xx}(x, t)}{w(x, t)} - \frac{1}{2} \left( \frac{w_x(x, t)}{w(x, t)} \right)^2 \right].
\]

As is seen, the function \( K(x, t) \) contains two contributions: in a sense, the first contribution has a 'corpuscular' nature, and the second is of a 'wave' nature. It is interesting to note that the expression for the second contribution is the same as for the Bohm 'quantum mechanical potential'. But in our approach, this contribution has a different physical meaning. Common to both approaches is the fact that the modulus of the wave function is related not only to probability.

Obviously, in the case of a spinless particle, for a quantum ensemble, one can introduce a field of any physical quantity \( O \) with a self-adjoint operator \( \hat{O} \):
\[
\langle O \rangle = \int_{-\infty}^{\infty} \psi^*(x, t) \hat{O} \psi(x, t) dx \equiv \int_{-\infty}^{\infty} O(x, t) w(x, t) dx; \quad O(x, t) = \frac{\text{Re} \left[ \psi^*(x, t) \hat{O} \psi(x, t) \right]}{\psi^*(x, t) \psi(x, t)}
\]
Therefore, the information inherent in the wave function about the physical properties of 'pure' quantum ensembles is much richer than it has been assumed until now.

Note, in order to experimentally verify the predictions of quantum mechanics regarding the properties of a pure quantum ensemble, there is no need to test all the fields that characterize it. For this, it is sufficient to investigate only the probability field \( w(x, t) \), which is related to the modulus of the wave function, and the momentum field \( p(x, t) \), which is related to its phase. Similarly, in the momentum representation we have the probability field \( w(p, t) \), the coordinate field \( x(p, t) \) and so on.

A special situation arises in those problems when the stationary states of the particle corresponding to the eigenvalues of the energy operator from the discrete spectrum are real. In this case, the phase of the wave function is zero. As a consequence, the field of pulses is also equal to zero, and the field of kinetic energy is determined only by the 'wave' term in (7).

2.2. Mixed state defined by superposition of pure states

Now consider a mixed state (11), which is a superposition of two pure states. Let the wave function \( \psi_1(x, t) \) define a (pure) quantum ensemble with a nonzero distribution function \( w_1(x, t) \) in the spatial domain \( G_1 \) and a momentum field \( p_1(x, t) \). Accordingly, let the wave function \( \psi_2(x, t) \) define a (pure) quantum ensemble with a nonzero distribution
function $w_2(x, t)$ in the spatial domain $G_2$ disjoint with the domain $G_1$, and field impulses $p_2(x, t)$.

Since both ensembles are localized in non-overlapping spatial regions, according to the separation principle, the state $|\Psi\rangle$ is mixed. This means that experimental verification of the predictions of quantum mechanics for this state is reduced to independent testing of the fields of pure states $\psi_1(x, t)$ and $\psi_2(x, t)$. It makes no physical sense to calculate the average values of physical quantities for the superposition of these two states.

### 2.3. Mixed state specified by the density operator

For comparison, now consider the mixed state, which is specified by the density operator

$$\hat{\rho} = c_1\ket{\psi_1}\bra{\psi_1} + c_2\ket{\psi_2}\bra{\psi_2},$$

where $c_1, c_2 \geq 0$, $c_1 + c_2 = 1$. In contrast to the previous case, we will assume that the pure states $\ket{\psi_1}$ and $\ket{\psi_2}$ are now localized in the same spatial region, but the designations for the probability field and the momentum field of each state will remain the same.

Now, when testing a quantum ensemble in state $\hat{\rho}$ at time $t$, with probability $c_1 \cdot w_1(x, t)dx$, we will find a particle in the interval $[x, x + dx]$ with momentum $p_1(x, t)$, and with probability $c_2 \cdot w_2(x, t)dx$ we will find it in the same interval with momentum $p_2(x, t)$. That is, in the case of a mixed ensemble given by the density operator $\hat{\rho}$, when measuring the momentum of a particle accidentally detected in the interval $[x, x + dx]$, now we can obtain (with probabilities $c_1$ and $c_2$) two values, and not one, as in the case of a pure state $|\Psi\rangle$ and a mixed state $|\Psi\rangle$ (in this case, the interval $[x, x + dx]$ can only belong to one of the regions $G_1$ and $G_2$).

### 3. Scattering a particle on a one-dimensional $\delta$-potential barrier in the context of “Einstein’s boxes”

Now let us study in more detail the connection between particle scattering on a one-dimensional $\delta$-potential barrier with the thought experiment “Einstein’s Boxes” and present a new model of this process.

#### 3.1. Stationary scattering states

Let us consider the $\delta$-potential $V(x) = W\delta(x)$ where $W > 0$ (there are no bound states). According to the SQM, the stationary Schrödinger equation can be written as

$$\hat{H}_{\text{tot}} \Psi_{\text{tot}}(x, k) \equiv -\frac{\hbar^2}{2m} \frac{d^2 \Psi_{\text{tot}}(x, k)}{dx^2} + W\delta(x)\Psi_{\text{tot}}(x, k) = E\Psi_{\text{tot}}(x, k);$$

where $k = \sqrt{2mE}/\hbar$ and $E$ is the particle energy; the Hamiltonian $\hat{H}_{\text{tot}}$ corresponds to the self-adjoint extension $\hat{H}_{\kappa,0}$ of the densely defined symmetrical operator $\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2}$ with $\text{Dom}(\hat{H}) = \{g \in H^{2,2}(\mathbb{R}) | g(0) = 0\}$ (see p.75 in [1]). The corresponding boundary conditions are

$$\Psi_{\text{tot}}(0^+) = \Psi_{\text{tot}}(0^-), \quad \Psi_{\text{tot}}'(0^+) - \Psi_{\text{tot}}'(0^-) = 2\kappa\Psi_{\text{tot}}(0^-);$$

where $\kappa$ is a parameter.
hereinafter, $\kappa = mW/\hbar^2$ and $f(0^\pm) = \lim_{\epsilon \to 0} f(\pm \epsilon)$ for any function $f(x)$; the prime denotes a derivative.

There are other two self-adjoint extensions of the operator $\hat{H}$ in the SQM. However, they are considered there as special cases corresponding to $\kappa = 0$ and $\kappa = \infty$ and, unlike $H_{\kappa,0}$, play the secondary role in this model. An intrigue is that in our approach we face with the opposite situation. We show that, in fact, these two special cases have no relation to $\kappa = 0$ and $\kappa = \infty$ and, unlike $H_{\kappa,0}$, play a key role (see Section 3.4) in the description of this scattering process.

The eigenvalues of the operator $\hat{H}_{\text{tot}}$ are doubly degenerate and lie in the domain $E \geq 0$. Thus, the general solution to the equation (8) with the boundary conditions (9) can be written as a linear superposition of two linearly independent particular solutions. As such, functions

$$\Psi_{L_{\text{tot}}}(x,k) = \begin{cases} e^{ikx} + A_{\text{ref}}(k)e^{-ikx}, & x < 0 \\ A_{\text{tr}}(k)e^{ikx}, & x > 0 \end{cases}$$

and

$$\Psi_{R_{\text{tot}}}(x,k) = \begin{cases} A_{\text{tr}}(k)e^{-ikx}, & x < 0 \\ e^{-ikx} + A_{\text{ref}}(k)e^{ikx}, & x > 0 \end{cases}$$

are usually taken, which describe a particle incident on the barrier from the left and right, respectively; here $A_{\text{tr}}(k) = k/(k + i\kappa)$, $A_{\text{ref}}(k) = -i\kappa/(k + i\kappa)$. The quantities $T(k) = |A_{\text{tr}}(k)|^2 = k^2/(k^2 + \kappa^2)$ and $R(k) = |A_{\text{ref}}(k)|^2 = \kappa^2/(k^2 + \kappa^2)$ represent the transmission and reflection coefficients, respectively (note that the transfer matrix for the delta potential can be obtained as the limiting transfer matrix of a rectangular potential barrier if the width of the barrier tends to zero and its area is fixed). As is seen, $T(0) = 0$. Therefore the functions $\Psi_{L_{\text{tot}}}(x,k)$ and $\Psi_{R_{\text{tot}}}(x,k)$ are identically zero for $k = 0$. Thus, the ground states are not involved in the construction of (non-stationary) scattering states – there are no particles with zero momentum in the quantum (one-particle) ensemble of particles incident on the barrier.

3.2. Scattering states with asymptotically free dynamics

Our next step is to find time-dependent solutions to the Schrödinger equation which would describe free dynamics in the limiting cases $t \to \mp \infty$. For only such states can be considered “scattering states”. For a particle incident on the barrier from the left, such states can be written in the form

$$\Psi_{L_{\text{tot}}}(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathcal{A}(k,t) \Psi_{L_{\text{tot}}}(x,k) dk;$$

where $\mathcal{A}(k,t) = \mathcal{A}_{\text{in}}(k) \exp[i(ka - E(k)t/\hbar)]$; a real function $\mathcal{A}_{\text{in}}(k)$ is such that the norm of the left asymptote

$$\Psi_{L_{\text{in}}}(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathcal{A}(k,t)e^{ikx} dk$$

is equal to one: $\int_{-\infty}^{\infty} |\mathcal{A}_{\text{in}}(k)|^2 dk = 1$. At the initial instant of time $t = 0$, the peak of the wave packet $\Psi_{L_{\text{in}}}(x,t)$ is located at the point $x = -a$. Accordingly, for a particle
incident on the barrier from the right, a time-dependent scattering state is

\[ \Psi^R_{tot}(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k, t) \Psi^R_{tot}(x, k) dk. \]  \hspace{1cm} (13)

In this case, the norm of the right in-asymptote

\[ \Psi^R_{in}(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k, t) e^{-ikx} dk \]  \hspace{1cm} (14)

is equal to one, and its peak is at the point \( x = +a \).

Let us consider, as \( A_{in}(k) \), the Gaussian function \( A_{in}(k) = \mathcal{A}_C(k) = c e^{-L^2(k-k_0)^2} \),
where \( c = \sqrt{\frac{2L^2}{\pi}} \), \( L \) is the width of the wave packet, in the \( k \)-space this wave packet is peaked at the point \( k_0 \). Strictly speaking, such a choice of the function \( A_{in}(k) \) does not meet the important requirement of the physical formulation of the scattering problem, since the wave packets (12) and (14) must be constructed only from waves that move towards the barrier. This means that \( A_{in}(k) \) must be nonzero only for \( k > 0 \). As will be shown below, the function \( \mathcal{A}_C(k) \) satisfies this condition only in some limiting cases.

According to the SQM (see [11 [16]), there is a strong limit in this scattering problem, and therefore the norms of \( \Psi^L_{tot}(x, t) \) and \( \Psi^R_{tot}(x, t) \), like the norms of their in-asymptotes, must be equal to one. Let us check this property by the example of the state (11) under the assumption that \( \mathcal{A}_{in}(k) \) is nonzero and for \( k \leq 0 \):

\[ \langle \Psi^L_{tot} | \Psi^L_{tot} \rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} [\mathcal{A}(k', t)]^* \mathcal{A}(k, t) I(k', k) dk' dk; \]

\[ I(k', k) = \lim_{X \to \infty} \tilde{I}(X, k', k); \quad \tilde{I}(X, k', k) = \int_{-X}^{X} [\Psi^L_{tot}(x, k')]^* \Psi^L_{tot}(x, k) dx. \]  \hspace{1cm} (15)

Substituting Exp. (10) for \( \Psi^L_{tot}(x, t) \) in (15), we get

\[ \tilde{I}(X, k', k) = \frac{2(k'k' + \kappa^2) + ik(k' - k)}{(k' - ik)(k + ik)} \sin[(k' - k)X] \frac{\sin[(k' + k)X]}{k' - k} - \frac{ik(k' - k - 2i\kappa)}{(k' - ik)(k + ik)} \frac{\sin[(k' + k)X]}{k' + k} + \frac{2\kappa}{(k' - ik)(k + ik)} \left[ \sin^2 \left( \frac{Xk' + k}{2} \right) - \sin^2 \left( \frac{Xk' - k}{2} \right) \right]. \]

Further, given that \( \lim_{X \to \infty} \frac{\sin(kX)}{k} = \pi \delta(k) \) and \( x\delta(x) = 0 \), we get

\[ I(k', k) = \frac{2(k'k' + \kappa^2) + ik(k' - k)}{(k' - ik)(k + ik)} \pi \delta(k' - k) - \frac{ik(k' - k - 2i\kappa)}{(k' - ik)(k + ik)} \pi \delta(k' + k) = 2\pi \delta(k' - k) - \frac{2i\kappa}{k + ik} \delta(k' + k). \]

Thus,

\[ \langle \Psi^L_{tot} | \Psi^L_{tot} \rangle = \int_{-\infty}^{\infty} [\mathcal{A}_{in}(k)]^2 dk - \int_{-\infty}^{\infty} \mathcal{A}_{in}(-k) \mathcal{A}_{in}(k) e^{2ika} \frac{ik}{k + ik} dk \]

\[ = \langle \Psi^L_{in} | \Psi^L_{in} \rangle + \kappa \int_{-\infty}^{\infty} \mathcal{A}_{in}(-k) \mathcal{A}_{in}(k) \frac{k \sin(2ka) - \kappa \cos(2ka)}{k^2 + \kappa^2} dk; \]  \hspace{1cm} (16)

here we took into account that \( \mathcal{A}_{in}(-k) \mathcal{A}_{in}(k) \) is an even real function. A similar situation arises in the case of the state (13).
Thus, \( \langle \Psi_{tot}^L | \Psi_{tot}^L \rangle = \langle \Psi_{in}^L | \Psi_{in}^L \rangle \) when \( A_{in}(-k)A_{in}(k) = 0 \). This takes place when \( A_{in}(k) \in C_0^\infty(\mathbb{R} \setminus \{0\}) = C_0^\infty(-\infty, 0) \oplus C_0^\infty(0, \infty) \), where \( C_0^\infty(-\infty, 0) \) and \( C_0^\infty(0, \infty) \) are the subspaces of infinitely differentiable functions which are identically zero on the semi-axises \([0, \infty)\) and \((-\infty, 0)\), respectively; for \( |k| \to 0 \) they tend to zero faster than \(|k|^n\); for \( |k| \to \infty \) they tend to zero faster than \(1/|k|^n\); \( n \) is a positive integer. With such functions \( A_{in}(k) \), solutions \( \Psi_{tot}^L(x, t) \) and \( \Psi_{tot}^R(x, t) \) of the time-dependent Schrödinger equation describe the scattering states with asymptotically free dynamics.

Another situation arises when \( A_{in}(k) \) is the Gaussian function \( A_G(k) \). Now (16) can be rewritten in the form

\[
\langle \Psi_{tot}^L | \Psi_{tot}^L \rangle = \langle \Psi_{in}^L | \Psi_{in}^L \rangle - \sqrt{2\pi\kappa L} \text{erfc} \left( \frac{2\kappa L^2 + a}{\sqrt{2L}} \right) e^{2L^2(k^2-k_0^2)+2\kappa a}. \tag{17}
\]

As is seen, the interference term is approximately zero when \( a/L \gg 1 \), \( L\kappa \gg 1 \), \( Lk_0 \gg 1 \). But if we also take into account that, at the initial instant of time, particles in the quantum ensemble must move towards the barrier, then the restrictions on the parameters of the Gaussian function \( A_{in}(k) \) will be written in the form \( a \gg L \gg 1/k_0 \). That is, the wave packets \( \Psi_{in}^L(x, t) \) and \( \Psi_{in}^R(x, t) \) should be quasi-monochromatic, and the width of each of these packets at \( t = 0 \) should be much less than the distance between the packet peak and the barrier.

### 3.3. A scattering particle with asymptotically free dynamics as an analogue of a particle in “Einstein boxes”

According to the SQM, each scattering state has one in-asymptote and one out-asymptote, and these asymptotes are not related to other scattering states. This property is satisfied when the Hamiltonian \( \hat{H}_{tot} \) is indeed self-adjoint (the corresponding quantum dynamics is unitary and (hence) unique). However, in this scattering problem, asymptotically free scattering states do not possess this property.

Consider the state \( \Psi_{tot}^L(x, t) \) with the Gaussian function \( A_{in}(k) \) for which the interference term in (17) is negligible. The advantage of making use of such states compared to scattering states with functions \( A_{in}(k) \) from the space \( C_0^\infty(\mathbb{R} \setminus \{0\}) \) is that in this case the wave function \( \Psi_{tot}^L(x, t) \) can be found in analytical form.

So, let \( A_{in}(k) = A_G(k) \) in (11). Then, taking into account (10), we obtain

\[
\Psi_{tot}^L(x, t) = \begin{cases} 
\Psi_{in}^L(x, t) - i\kappa G(-x, t); & x < 0 \\
\Psi_{in}^L(x, t) - i\kappa G(x, t); & x > 0 
\end{cases} \tag{18}
\]

where \( \Psi_{in}^L(x, t) \) is the in-asymptote (see (12))

\[
\Psi_{in}^L(x, t) = \frac{c}{\sqrt{2(L^2 + ibt)}} \exp \left( \frac{-(x+a)^2 + 4ik_0L^2(x+a-bk_0t)}{4(L^2 + ibt)} \right). \tag{19}
\]

\( b = \hbar/(2m) \); and

\[
G(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k, t) \frac{e^{ik(x+a)}}{k + i\kappa} dk. \tag{20}
\]
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The integral \( G(x, t) \) can be found as a solution to the equation

\[
\frac{\partial G(x, t)}{\partial x} = \kappa G(x, t) + i\Psi_L(x, t)
\]

which follows from (20). It can be shown that

\[
G(x, t) = -ic\sqrt{\frac{\pi}{2}} \text{erfc} \left( \frac{x + a - 2iL^2k_0}{2\sqrt{L^2 + ibt}} \right) e^{t^2(\kappa - ik_0)^2 + ib\kappa^2 + \kappa(x + a)}. \tag{21}
\]

For what follows, we also need the integral

\[
F(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k, t) \frac{e^{ik(x + a)}}{k - i\kappa} dk. \tag{22}
\]

It is easy to show that

\[
F(x, t) = i\kappa \sqrt{\frac{\pi}{2}} \text{erfc} \left( \frac{-x + a - 2iL^2k_0}{2\sqrt{L^2 + ibt}} \right) e^{t^2(\kappa + ik_0)^2 + ib\kappa^2 - \kappa(x + a)}. \]

Now we have, in analytical form, not only the scattering state (18) itself and its in-asymptote (19), but also its out-asymptote which represents a superposition

\[
\Psi_{\text{out}}(x, t) = \Psi_{\text{in}}^L(x, t) + \Psi_{\text{out}}^R(x, t) \tag{23}
\]

of the left and right asymptotes \( \Psi_{\text{out}}^L(x, t) \) and \( \Psi_{\text{out}}^R(x, t) \),

\[
\Psi_{\text{out}}^L(x, t) = -i\kappa G(-x, t), \quad \Psi_{\text{out}}^R(x, t) = \Psi_{\text{in}}^L(x, t) - i\kappa G(x, t), \tag{24}
\]

localized in the non-intersecting spatial regions lying on the opposite sides of the barrier.

According to the SQM, only the scattering state (18) is related to this asymptote. But this is not the case. Let us consider the family of the stationary states

\[
\Psi(x, k; \lambda) = \Psi_{\text{tot}}^L(x, k) + (e^{i\lambda} - 1)\tilde{\Psi}(x, k) \tag{25}
\]

with different values of the parameter \( \lambda \), where

\[
\tilde{\Psi}(x, k) = \begin{cases} 
\frac{k^2}{k + ik}\rho_{ik}e^{ikx}; & x < 0 \\
\frac{e^{ikx}}{k + ik}\rho_{ik}; & x > 0
\end{cases}
\]

The corresponding scattering states built with the Gaussian function \( A_G(k) \) are

\[
\Psi(x, t; \lambda) = \Psi_{\text{tot}}^L(x, t) + (e^{i\lambda} - 1)\tilde{\Psi}(x, t), \tag{26}
\]

where

\[
\tilde{\Psi}(x, t) = \begin{cases} 
\Psi_{\text{in}}^L(x, t) - \frac{i\kappa}{2}[G(x, t) - F(x, t)]; & x < 0 \\
\Psi_{\text{in}}^L(x, t) - i\kappa G(x, t) + \frac{i\kappa}{2}[G(-x, t) + F(-x, t)]; & x > 0
\end{cases}
\]

Their out-asymptotes (coinciding at \( \lambda = 0 \) with the out-asymptote (23)) are

\[
\Psi_{\text{out}}(x, t; \lambda) = \Psi_{\text{out}}^L(x, t) + e^{i\lambda}\Psi_{\text{out}}^R(x, t), \tag{27}
\]

localized, in the limit \( t \to \infty \), in the disjoint spatial regions lying on the opposite sides of the barrier. That is, this situation is similar to the one that occurs in “Einstein’s boxes”.

Due to the barrier region that separates the out-asymptotes \( \Psi_{\text{out}}^L(x, t) \) and \( \Psi_{\text{out}}^R(x, t) \) in the limit \( t \to \infty \), the mean value of any observable does not depend on the phase
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$\lambda$ (of course, this property is strictly fulfilled only for $A_{m}(k) \in C_{0}^{\infty}(\mathbb{R}\{0\}))$. This is demonstrated on fig. 1 by the example of the average value of the position operator, calculated for the state $\Psi_{out}(x,t;\lambda)$ at $\lambda = 0$, $\lambda = \pi/2$ and $\lambda = \pi$; making use of the units $\hbar = m = 1$, we take $\kappa = 1$, $L = 5$, $a = 30$ and $k_{0} = 0.5$. It should be stressed that the interference term in (17) is negligible in this case.

![Figure 1.](image-url)

In the limiting case $t \to \infty$, for the out-asymptote (27) it is valid the averaging rule

$$\langle \Psi_{out} | x | \Psi_{out} \rangle \equiv \langle x \rangle_{out} = \langle T \rangle \cdot \langle x \rangle_{out}^{R} + \langle R \rangle \cdot \langle x \rangle_{out}^{L}$$

which says that $\lambda$ is unobserved and the state (27) is mixed; here

$$\langle x \rangle_{out}^{R} = \frac{\langle \Psi_{out}^{R} | x | \Psi_{out}^{R} \rangle}{\langle \Psi_{out}^{R} | \Psi_{out}^{R} \rangle}, \quad \langle x \rangle_{out}^{L} = \frac{\langle \Psi_{out}^{L} | x | \Psi_{out}^{L} \rangle}{\langle \Psi_{out}^{L} | \Psi_{out}^{L} \rangle}; \quad T = \langle \Psi_{out}^{R} | \Psi_{out}^{R} \rangle, \quad R = \langle \Psi_{out}^{L} | \Psi_{out}^{L} \rangle;$$

$T$ and $R$ are the transmission and reflection coefficients.

So, for a particle that falls on the barrier from the left and is described by a wave function (13), in the limit $t \to \infty$, exactly the same situation arises as for a particle in the experiment with two boxes. The 'boxes' here are the intervals $(-\infty, 0)$ and $(0, \infty)$; the out-asymptote $\Psi_{out}^{L}(x,t)$, which describes reflected particles, is localized in the left 'box', and the out-asymptote $\Psi_{out}^{R}(x,t)$, which describes the transmitted particles, is localized in the right 'box'. Thus, the superposition of these two (pure) out-asymptotes, localized in independent 'boxes', is a mixed state (analogous to the state (1)). And since this 'mixed' out-asymptote is common for the entire one-parameter class of states $\Psi(x,t;\lambda)$ given by the expression (26), we come to the conclusion that all non-stationary states (26) are mixed states at $t \to \infty$.

Note that the states $\Psi(x,t;\lambda)$ (26) at $\lambda \neq 0$ describe scattering processes with two-sided incidence of a particle on a barrier. In this case, the analogy with two boxes
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arises not only in the limit $t \to \infty$, but also in the limit $t \to -\infty$. Thus, the states $\Psi(x,t;\lambda)$ for $\lambda \neq 0$ are mixed ones also for $t \to \infty$.

As for the state $\Psi(x,t;0) = \Psi^L_{tot}(x,t)$, which describes the scattering problem with a left-hand fall of a particle onto a barrier, its in-asymptote $\Psi^L_{in}(x,t)$ is a pure state. Thus, a situation arises that is paradoxical for the Schrodinger formalism – the nonstationary scattering state $\Psi^L_{tot}(x,t)$ interpolates between the pure in-asymptote $\Psi^L_{in}(x,t)$ and the superposition of two independent out-asymptotes $\Psi^L_{out}(x,t)$ and $\Psi^R_{out}(x,t)$, which is a mixed state.

Such Schrodinger dynamics could be viewed as a transition of a closed system from a pure state to a mixed one (see section 1.3). But, as shown above, this dynamics ceases to be unambiguous when $t \to \infty$. Therefore, it is not unitary, which means that the operator $\hat{H}_{tot}$ is not self-adjoint, and no observable can be defined for the entire scattering process. In other words, the unsteady state of scattering $\Psi(x,t;0)$ (that is, $\Psi^L_{tot}(x,t)$) is a mixed state, and the process itself with a left-hand fall of a particle onto a barrier is a mixture of two sub-processes – transmission and reflection. In this regard, it becomes necessary to reconstruct the entire prehistory of the transmitted and reflected wave packets to describe the subprocesses at all stages of scattering.

As shown in [17] using a rectangular potential barrier as an example, for any one-dimensional short-range potential barrier this prehistory can be reconstructed uniquely by the in-asymptote $\Psi^L_{in}(x,t)$, which describes the entire ensemble of particles, and out-asymptotes $\Psi^L_{out}(x,t)$ and $\Psi^R_{out}(x,t)$ that describing sub-ensembles of transmitted and reflected particles (this idea is also applicable to the potential step). In the case of the $\delta$-potential, a modification of this approach is possible, which we present in the next two sections.

3.4. Self-adjoint extensions associated with the 'periodic' and Dirichlet boundary conditions

Let us consider the presented in [1] two 'special cases' of self-adjoint extensions of the operator $\hat{H}$. One of them involves the periodic boundary conditions

$$\psi(0^+) = \psi(0^-), \quad \psi'(0^+) = \psi'(0^-).$$

The corresponding (self-adjoint) Hamiltonian $\hat{H}_0$ (see [1]) will be also denoted by $\hat{H}_{tr}$:

$$\hat{H}_{tr} = \hat{H}_0 = -\frac{d^2}{dx^2}; \quad \text{Dom}(\hat{H}_0) = W^2_2(\mathbb{R}).$$

Note that $\hat{H}_0 \neq \lim_{\kappa \to 0} H_{\kappa,0}$ because $\text{Dom}(H_{\kappa,0}) \neq \text{Dom}(\hat{H}_0)$ at any arbitrary small value of $\kappa > 0$. For a free particle, two independent solutions of the corresponding stationary Schrödinger equation are

$$\Psi^L_{tr}(x,k) = e^{ikx}, \quad \Psi^R_{tr}(x,k) = e^{-ikx}, \quad x \in (-\infty, \infty).$$

Another 'special case' is associated with the Dirichlet boundary conditions

$$\psi(0^+) = \psi(0^-) = 0.$$
The corresponding self-adjoint extension of $\hat{H}$ will be denoted by $\hat{H}_{\text{ref}}$. Note (see also [11]), the boundary conditions (31) do not impose any restrictions on the derivatives $\psi'(0^+)$ and $\psi'(0^-)$, thereby totally disconnecting the $x$-intervals $(-\infty, 0)$ and $(0, \infty)$. Thus, $\hat{H}_{\text{ref}} \neq \lim_{\kappa \to \infty} \hat{H}_{\kappa,0}$ because the boundary conditions [9] do not disconnect these intervals even in the limit $\kappa \to \infty$. So,

$$\hat{H}_{\text{ref}} = \hat{H}_{\text{ref}}^L \oplus \hat{H}_{\text{ref}}^R,$$

and the eigenfunctions of the operators $\hat{H}_{\text{ref}}^L$ and $\hat{H}_{\text{ref}}^R$ are defined on the semi-axes $(-\infty, 0)$ and $(0, \infty)$, respectively. Solutions to the corresponding stationary Schrödinger equations are

$$\Psi_{\text{ref}}^L(x,k) = e^{ikx} - e^{-ikx}, \quad x < 0; \quad \Psi_{\text{ref}}^R(x,k) = e^{-ikx} - e^{ikx}, \quad x > 0. \quad (33)$$

### 3.5. Scattering states as coherent superpositions of transmission and reflection states

Let us now show that the state $\Psi_{\text{tot}}^L(x,k)$ can be uniquely represented as a superposition of the states $\Psi_{\text{tr}}^L(x,k)$ and $\Psi_{\text{ref}}^L(x,k)$. For this purpose, let us write the incident wave of the state $\Psi_{\text{tot}}^L(x,k)$ as a superposition of two incident waves, with the amplitudes $A_{\text{in}}^\text{tr}(k)$ and $A_{\text{in}}^\text{ref}(k)$, associated with the states $\Psi_{\text{tr}}^L(x,k)$ and $\Psi_{\text{ref}}^L(x,k)$, respectively. In this case, we will assume that $A_{\text{in}}^\text{tr}(k) = |A_{\text{tr}}^\text{in}(k)| e^{i\mu(k)}$ and $A_{\text{in}}^\text{ref}(k) = |A_{\text{ref}}^\text{in}(k)| e^{i\nu(k)}$. Real phases $\mu$ and $\nu$ obey the equation $\sqrt{T(k)} |e^{i\mu(k)} + \sqrt{R(k)} e^{i\nu(k)}| = 1$ which has two roots

$$\nu(k) = \mu(k) - \frac{\pi}{2}, \quad \mu(k) = \pm \text{arctan} \left( \frac{\sqrt{R(k)}}{T(k)} \right), \quad (34)$$

the corresponding amplitudes are

$$A_{\text{in}}^\text{tr} = \sqrt{T} (\sqrt{T} \pm i \sqrt{R}) = \frac{k(k \pm i\kappa)}{k^2 + \kappa^2}, \quad A_{\text{in}}^\text{ref} = \sqrt{R} (\sqrt{R} \pm i \sqrt{T}) = \frac{\kappa(\kappa \pm i\kappa)}{k^2 + \kappa^2}. \quad (36)$$

It is seen that $A_{\text{in}}^\text{tr} = A_{\text{tr}}^\text{in}$ and $A_{\text{in}}^\text{ref} = -A_{\text{ref}}^\text{in}$, for the lower sign; while $A_{\text{in}}^\text{tr} = A_{\text{tr}}^\text{in}$ and $A_{\text{in}}^\text{ref} = -A_{\text{ref}}^\text{in}$, for the upper sign. For both roots $A_{\text{in}}^\text{tr} + A_{\text{in}}^\text{ref} = 1$ and $|A_{\text{in}}^\text{tr}|^2 + |A_{\text{in}}^\text{ref}|^2 = 1$.

Considering only amplitudes corresponding to the lower sign, it is easy to show that the function $\Psi_{\text{tot}}^L(x,k)$ can be uniquely written as a superposition of the states $\Psi_{\text{tr}}^L(x,k)$ and $\Psi_{\text{ref}}^L(x,k)$:

$$\Psi_{\text{tot}}^L(x,k) = A_{\text{in}}^\text{tr}(k) \Psi_{\text{tr}}^L(x,k) + A_{\text{in}}^\text{ref}(k) \Psi_{\text{ref}}^L(x,k) \quad (35)$$

(the amplitudes $A_{\text{in}}^\text{tr}$ and $A_{\text{in}}^\text{ref}$ which correspond to the upper sign in Exp. (34) appear in the expressions complex conjugate to Exps. (35)). Similarly, for the right incidence

$$\Psi_{\text{tot}}^R(x,k) = A_{\text{in}}^\text{tr}(k) \Psi_{\text{tr}}^R(x,k) + A_{\text{in}}^\text{ref}(k) \Psi_{\text{ref}}^R(x,k).$$

Thus, as it follows from (35), the time-dependent scattering states $\Psi_{\text{tot}}^L$ and $\Psi_{\text{tot}}^R$ can be uniquely written as coherent superpositions

$$\Psi_{\text{tot}}^L(x,t) = \Psi_{\text{tr}}^L(x,t) + \Psi_{\text{ref}}^L(x,t), \quad \Psi_{\text{tot}}^R(x,t) = \Psi_{\text{tr}}^R(x,t) + \Psi_{\text{ref}}^R(x,t), \quad (36)$$
In particular, for the left incidence with the Gaussian function $A_{\text{in}}(k)$ where $L$ from the in-asymptote $\Psi_{\text{in}}(x,t)$ conditional probabilities). And since the dynamics of both subprocesses is restored work [2, 3], where the problem of indirect measurement is based on the formalism of impossibility of directly measuring the characteristic times is also emphasized in the obvious, this also applies to the determination of their characteristic times (the scattering state $\Psi_{\text{tot}}(x,t)$ with Gaussian in-asymptote $\Psi_{\text{in}}(x,t)$, describing the scattering process with by left-hand fall of a particle on a barrier, can be written at all stages of scattering as a superposition (36) of two pure states $\Psi_{\text{tr}}(x,t)$ and $\Psi_{\text{ref}}(x,t)$ with norms $\sqrt{T}$ and $\sqrt{R}$, respectively. This superposition has properties unusual for the Schrodinger formalism: it is a mixed state, although the states $\Psi_{\text{tr}}(x,t)$ and $\Psi_{\text{ref}}(x,t)$ separated only in the limit $t \to \infty$. At the previous stages, in the region $x < 0$, they overlap and interfere with each other.

All this means that an experimental study of the transmission and reflection subprocesses in this area is possible only with the help of indirect measurements. Obviously, this also applies to the determination of their characteristic times (the impossibility of directly measuring the characteristic times is also emphasized in the work [2, 3], where the problem of indirect measurement is based on the formalism of conditional probabilities). And since the dynamics of both subprocesses is restored from the in-asymptote $\Psi_{\text{in}}(x,t)$ and the out-asymptote $\Psi_{\text{out}}(x,t)$ and $\Psi_{\text{out}}(x,t)$, wave functions $\Psi_{\text{tr}}(x,t)$ and $\Psi_{\text{ref}}(x,t)$ for $x < 0$ should be written in terms of these asymptotes, extending their dynamics to the whole time-axis.

Using Exps. (38), we get

$$\Psi_{\text{tr}}(x,t) = \Psi_{\text{in}}(x,t) + \Psi_{\text{out}}(x,t), \quad \Psi_{\text{ref}}(x,t) = \Psi_{\text{ref}}(x,t) - \Psi_{\text{out}}(x,t). \quad (39)$$

Then, passing to the (normalized to unity) wave functions $\tilde{\Psi}_{\text{tr}}(x,t) = \Psi_{\text{tr}}(x,t)/\sqrt{T}$ and $\tilde{\Psi}_{\text{ref}}(x,t) = \Psi_{\text{ref}}(x,t)/\sqrt{R}$, we calculate (in accordance with Section 2.1) the corresponding probability fields $w_{\text{tr}}(x,t)$ and $w_{\text{ref}}(x,t)$, as well as the momentum fields $p_{\text{tr}}(x,t)$ and $p_{\text{ref}}(x,t)$.

It is interesting to compare these functions with the corresponding fields $w_{\text{tot}}(x,t)$ and $p_{\text{tot}}(x,t)$, which describe the whole process. Calculations are performed for the
in-asymptote $\Psi_{\text{in}}^L(x,t)$ (see (19)) with parameters corresponding to fig. 1 for $\lambda = 0$. In this case $T \approx 0.2$ and $R \approx 0.8$. For the very in-asymptote (19))

\[
\begin{align*}
    p_{\text{in}}^L(x,t) &= \frac{2L^4k_0 + (a + x)bt}{2(L^4 + b^2t^2)}, \\
    w_{\text{in}}^L(x,t) &= \frac{c^2}{2\sqrt{L^4 + b^2t^2}} \exp \left( \frac{-L^2(x + a - 2k_0bt)^2}{2(L^4 + b^2t^2)} \right). \tag{40}
\end{align*}
\]

It easy to check that $\int_{-\infty}^{\infty} p_{\text{in}}^L(x,t) w_{\text{in}}^L(x,t) dx = \hbar k_0$.

Figs. 2 and 3 show the calculation results for $t = 0$. As expected, at the initial

![Figure 2](image2.png)

**Figure 2.** $w_{\text{tot}}^L(x,0)$ (dotted line), $w_{\text{tr}}^L(x,0)$ (dashed line) and $w_{\text{ref}}^L(x,0)$ (solid line).

![Figure 3](image3.png)

**Figure 3.** $p_{\text{tot}}^L(x,0)$ (dotted line), $p_{\text{tr}}^L(x,0)$ (dashed line) and $p_{\text{ref}}^L(x,0)$ (solid line).
in the same spatial region. At all points of this region $p_{tr}^L(x,0) > p_{tot}^L(x,0) > p_{ref}^L(x,0)$, which was also natural to expect.

The calculation results for $t = 60$ are shown in figs. 4 and 5.

4. Discussion and conclusions

It is shown that the problem of scattering a particle by a one-dimensional $\delta$-potential is an analogue of the thought experiment with two boxes, which Einstein used against
the orthodox doctrine of the completeness of quantum mechanics. In this regard, we presented our vision of this experiment. From our analysis it follows that the separation principle, formulated by Einstein, is directed not so much against this doctrine (for this it is enough to consider the experiment with one box), how much against the existing formulation of the principle of superposition, according to which the state of a particle in boxes independent from each other should be considered as a pure quantum state. Moreover, this formulation contradicts not only Einstein’s separation principle, but also the definition of mixed states of quantum mechanics itself. Thus, orthodox quantum mechanics is internally contradictory and requires a correction of the superposition principle when describing quantum one-particle dynamics, during which “Einstein boxes” arise (i.e., when states localized in spatial regions separated by an infinitely deep potential well). Apart from the scattering problem considered, such a situation arises in the model \[18\] of a one-dimensional hydrogen atom.

In the investigated scattering problem, “Einstein’s boxes” arise when \( t \to \infty \). In this limit, the scattering states with asymptotically free dynamics lose the property of uniqueness and, therefore, develop in time in a non-unitary manner. In other words, the formal Hamilton operator with \( \delta \)-potential is a non-self-adjoint operator, and the scattering process with one-sided incidence of a particle on the barrier is a mixture of two subprocesses – transmission and reflection. An approach is presented for recovering the wave functions that describe these subprocesses, by the in-asymptote of the entire process and the out-asymptotes describing the subprocesses. Based on these functions, it is possible to indirectly measure the physical characteristics of each of their subprocesses for the first stages of scattering.

Note that the question of the physical aspects of quantum dynamics in this scattering problem is solved, in our approach, on the basis of new idea about the physical properties of a pure quantum ensemble, specified by the wave function. According to modern quantum mechanics, the wave function imposes only statistical restrictions on the properties of the ensemble. But this is far from the case. First, through the square of the modulus of the wave function (in the coordinate representation), not only the distribution function of particles over coordinates (the ‘probability field’ of the ensemble) is determined, but also its kinetic-energy field. Second, the phase of the wave function has a physical meaning too – it sets the momentum field of the ensemble. In this one-dimensional scattering problem, all these fields are functions of two independent variables \( x \) and \( t \) (or, \( p \) and \( t \), in the momentum representation).

In other words, quantum mechanics not only does not prohibit the simultaneous measurement of the coordinate and momentum of a particle (as well as kinetic energy), but also predicts the value of the momentum at that spatial point where the particle will be (accidentally) detected. And this in no way contradicts the Heisenberg uncertainty principle, which imposes restrictions on the standard deviations of the coordinates of particle momenta in a quantum ensemble, and not on the measurement errors of these quantities.

The fact that the wave function predicts the fields of physical quantities that
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characterize a quantum ensemble suggests that its physical properties are uniquely determined by external physical conditions (macroscopic physical context) under which each member of the ensemble moves. We have also to note that the sets of fields in the $x$- and $p$-representations are different: in the first case we have the $w(x,t)$-, $p(x,t)$- and $K(x,t)$-fields and so on; in the second case we have the $w(p,t)$-, $x(p,t)$- and $x^2(p,t)$-fields and so on.

References

[1] Albeverio S., Gesztesy F., Høegh-Krohn R., Holden H. (with appendix written by P. Exner) Solvable models in quantum mechanics, AMS Chelsea Publishing, 2000.
[2] Aephraim M. Steinberg, Conditional probabilities in quantum theory and the tunneling-time controversy. Phys.Rev. A. 52, 32-42 (1995)
[3] David C. Spierings and Aephraim M. Steinberg, Observation of the Decrease of Larmor Tunneling Times with Lower Incident Energy. Phys.Rev. Lett. 127, 133001 (2021)
[4] Arthur Fine, “The Shaky Game” (The University of Chicago Press, 1986),
[5] L. E. Ballentine, “Einstein’s Interpretation of Quantum Mechanics”, American Journal of Physics 40, 1763(1972); doi: 10.1119/1.1987060
[6] D. Howard, “Einstein on locality and separability.” Stud. Hist. Phil. Set., Vol. 16, No. 3, pp. 171–201, 1985.
[7] Travis Norsen, “Einstein’s Boxes.” American Journal of Physics 73, 164 (2005); https://doi.org/10.1119/1.1811620
[8] Carsten Held, “Einstein’s Boxes: Incompleteness of Quantum Mechanics Without a Separation Principle”, Found Phys (2015) 45:1002-1018 DOI 10.1007/s10701-014-9845-6
[9] Jean Bricmont, “History of Quantum Mechanics or the Comedy of Errors”, [arXiv:1703.00294v1 [physics.hist-ph]]
[10] Bogdan Mielnik, “The Paradox of Two Bottles in Quantum Mechanics”, Foundations of Physics, Vol. 20, No. 6, 745–755, 1990
[11] B Mielnik, “Empty Bottle: The Revenge of Schrödinger’s Cat?”. IOP Conf. Series: Journal of Physics: Conf. Series 839 (2017) 012006 doi :10.1088/1742-6596/839/1/012006
[12] Leslie Ballentine, “The Statistical Interpretation of Quantum Mechanics”, Rev. of Modern Phys. (1970) 42: 358-381
[13] J.S. Bell, “Speakable and unspeakable in quantum mechanics”, Cambridge University Press, 1987.
[14] D. Bohm, “A Suggested Interpretation of the Quantum Theory in Terms of ”Hidden” Variables. I”, Phys. Rev. v.85, (1952) 166-179.
[15] D. Bohm, “A Suggested Interpretation of the Quantum Theory in Terms of ”Hidden” Variables. II”, Phys. Rev. v.85, (1952) 180-193.
[16] Reed M. and Simon B. Methods of modern mathematical physics. III: Scattering theory, Academic Press, Inc., 1979.
[17] Nikolay L. Chuprikov, From a 1D Completed Scattering and Double Slit Diffraction to the Quantum-Classical Problem for Isolated Systems. Found Phys (2011) 41:1502-1520 DOI 10.1007/s10701-011-9564-1
[18] H. N. Nunez Ypez et al, “Superselection rule in the one-dimensional hydrogen atom”, J. Phys. A: Math. Gen. 21, L651–L653 (1988)