N. L. Chuprikov

Revising the applicability of the Stone-von Neumann theorem to scattering a quantum particle on a one-dimensional potential barrier

Received: date / Accepted: date

Abstract It is shown that the Stone-von Neumann theorem is inapplicable to scattering a quantum nonrelativistic particle on a one-dimensional "short-range" potential barrier, since the unboundedness of the position operator plays here a crucial role. The Shrödinger representation associated with this process is reducible: long before and long after the scattering event the space of its asymptotes represents the direct sum of the subspaces of left and right asymptotes. There is a dichotomous-context-induced superselection rule (SSR), in which the role of a superselection operator is played by the Pauli matrix $\sigma_3$ and the role of superselection (coherent) sectors is played by the above subspaces. By the SSR any superposition of states from different coherent sectors is a mixed state, and splitting the incident wave packet into the transmitted and reflected parts is nothing but a conversion of a pure state into a mixed one. The average values of any observable can be defined only for the transmission and reflection subprocesses. The former evolves within a single coherent sector of the Hilbert space, in the momentum representation; while the latter evolves within a single coherent sector of this space, in the coordinate representation.

Keywords one-dimensional scattering · Stone-von Neumann theorem · superselection rule

1 Introduction

The main goal of this paper is revising the contemporary quantum model (CQM) of scattering a nonrelativistic particle on a one-dimensional (1D) potential barrier with support within some bounded spatial interval. This model is presented in many textbooks on quantum mechanics as an example of an internally consistent quantum theory. However, in fact, this is not the case.

Let $\hat{H}$ be Hamiltonian that describes scattering a particle on the "short-range" potential $V(x)$ which is nonzero in the interval $[-a,a]$ (in order to focus all our attention on the main issue, we will assume that $\hat{H}$ has no bound states), and $|\psi_0\rangle$ be the initial state of a particle. Then, according to the CQM (see, e.g., [1–4]), the basic properties of this one-particle process can be expressed in the following statements:

a) There are in and out asymptotes $|\psi_{\text{in}}\rangle$ and $|\psi_{\text{out}}\rangle$ such that the scattering state $e^{-i\hat{H}t/\hbar}|\psi_0\rangle$ ”interpolates” between them. The left and right parts of each asymptote are localized in the non-overlapping spatial regions that lie on different sides of the barrier – long before and long after the scattering event, i.e., when $t \to \mp\infty$, a particle does not interact with the "short-range" potential.

b) Both asymptotes are uniquely determined by the initial state of a particle: $|\psi_{\text{in}}\rangle = \hat{\Omega}_+|\psi_0\rangle$ and $|\psi_{\text{out}}\rangle = \hat{\Omega}_-|\psi_0\rangle$, where $\hat{\Omega}_\pm = \lim_{t \to \pm\infty} e^{i\hat{H}t/\hbar} e^{-i\hat{H}_0t/\hbar}$ are the in and out Møller wave operators; $\hat{H}_0$ is the free one-particle Hamiltonian.
c) The space $\mathcal{H}_{in}$ of in asymptotes and the space $\mathcal{H}_{out}$ of out asymptotes coincide with each other: $\mathcal{H}_{in} = \mathcal{H}_{out} = \mathcal{H}_{as}$ (weak asymptotic completeness). Moreover, in the case considered, that is, when $\mathcal{H}$ has no bound states, $\mathcal{H}_{as}$ spans the entire Hilbert space $\mathcal{H}$, that is, $\mathcal{H}_{as} = \mathcal{H}$.

d) The Schrödinger representation is irreducible and, thus, $\mathcal{H}_{as}$ can not be presented as a direct sum of nontrivial subspaces which would be invariant for the position and momentum operators. This also means that any asymptotic state from $\mathcal{H}_{as}$ is a pure state, and a superposition of any two asymptotic states from $\mathcal{H}_{as}$ is another pure state from $\mathcal{H}_{as}$.

e) There is a linear unitary transformation $S = \hat{\Omega}_{L,\Omega}$ which "correlates the past and future asymptotics of interacting histories" [1]: $|\psi_{out}\rangle = S|\psi_{in}\rangle$. "The fact that $S$ is unitary means that for every normalized $|\psi_{in}\rangle$ there is a unique normalized $|\psi_{out}\rangle$ and vise versa; and also (because $S$ is linear) that the correspondence between $|\psi_{in}\rangle$ and $|\psi_{out}\rangle$ preserves superposition, that is, if $|\psi_{in}\rangle = a|\phi_{in}\rangle + b|\chi_{in}\rangle$, then $|\psi_{out}\rangle = a|\phi_{out}\rangle + b|\chi_{out}\rangle"$ [3] p.36.

Note that the statement (d) is, perhaps, most fundamental here, because the irreducibility of the Schrödinger representation guarantees the validity of the superposition principle in the space $\mathcal{H}$. Nevertheless, namely this statement makes this model internally inconsistent and must be discarded from this list, because it contradicts the item (a) and is based on the erroneous assumption that the Stone-von Neumann theorem is applicable to this scattering process.

As is known (see, e.g., [2][3]), in the Stone-von Neumann theorem the position operator is treated like bounded operators. At the same time the unboundedness of this operator plays a crucial role in the problem under study: the item (a) implies that, in the limits $t \rightarrow \pm \infty$, a particle does not interact with the barrier and the space $\mathcal{H}_{as}$ represents a direct sum of the non-overlapping subspaces of left and right asymptotes. Making use of Hall’s terminology (see [3] p.281), we can say that in the case of this process we meet just with that "bad" case of the canonical commutation relations, which is not covered by the Stone-von Neumann theorem.

As will be shown below, the dichotomous physical context, formed by the different physical conditions on either side of the barrier, induces a superselection rule (SSR), according to which the left and right asymptotes belong to different coherent (superselection) sectors of the Hilbert space $\mathcal{H}_{as}$ when $t \rightarrow \pm \infty$. These subspaces are invariant for the position and momentum operators, as well as for the Pauli matrix $\sigma_a$ that plays in this space the role of a superselection operator. By this rule a superposition of left and right asymptotes represents a mixed state, rather than a pure one.

2 Stationary states of a particle in the formalism of the transfer and scattering matrices.

We begin our analysis with solving the stationary Schrödinger equation for a particle with a given energy $E = (\hbar k)^2/2m$; $m$ is its mass. In the general case the wave function $\Psi(x;k)$, beyond the interval $[-a,a]$, can be written in the form

$$\Psi(x;k) = \begin{cases} A_{L,in}(k) e^{ikx} + A_{L,out}(k) e^{-ikx}, & x \leq -a; \\ A_{R,in}(k) e^{ikx} + A_{R,out}(k) e^{-ikx}, & x \geq +a \end{cases}$$

(1)

Its amplitudes in the regions $x \leq -a$ and $x \geq a$ are linked by the transfer matrix $Y(k)$:

$$\begin{pmatrix} A_{L,in} \\ A_{L,out} \end{pmatrix} = Y \begin{pmatrix} A_{R,out} \\ A_{R,in} \end{pmatrix}; \quad Y = \begin{pmatrix} q & p \\ p^* & q^* \end{pmatrix};$$

(2)

where $q(-k) = q^*(k)$, $p(-k) = p^*(k)$. According to [3], for any potential barrier with support inside $[x_1,x_2]$ the transfer-matrix elements can be written as follows,

$$q = \frac{1}{\sqrt{T(k)}} e^{i[k(x_2-x_1)-J(k)]}, \quad p = i \sqrt{\frac{R(k)}{T(k)}} e^{i[-k(x_2+x_1)+F(k)]}, \quad R = 1 - T;$$

(3)

$T(-k) = T(k)$, $J(-k) = J(k)$, $F(-k) = \pi - F(k)$; for the case considered $x_2 - x_1 = d = 2a$ and $x_2 + x_1 = 0$. For any symmetric potential barrier, $V(-x) = V(x)$, the phase $F$ takes only two values: 0 or $\pi$. In this case, a piecewise-constant function $F(k)$ has discontinuities at the points where the reflection coefficient equals to zero.
Note that the scattering parameters (the transmission $T$ and reflection $R$ coefficients, as well as the phases $J$ and $F$) can be calculated (analytically or numerically) for potential barriers of any form. For this purpose one can use either analytical expressions in [3], if $V(x)$ is the rectangular potential barrier or the δ-potential, or recurrence relations, if $V(x)$ represents a system of δ-potentials and piecewise continuous potential barriers. Thus, we can further assume that the matrix $Y(k)$ and the scattering matrix $S$ that links the amplitudes $A_{L,\text{out}}$ and $A_{R,\text{out}}$ of outgoing waves with the amplitudes $A_{L,\text{in}}$ and $A_{R,\text{in}}$ of incoming waves are known.

Since this link can be realized in two ways, and both will be important for our approach (see Section 3), we consider two scattering matrices $-S_k$ and $S_x$:

$$
\begin{pmatrix}
A_{R,\text{out}} \\
A_{L,\text{out}}
\end{pmatrix}
= S_k
\begin{pmatrix}
A_{L,\text{in}} \\
A_{R,\text{in}}
\end{pmatrix},
S_k = \frac{1}{q} \begin{pmatrix} 1 & -p \\ p^* & 1 \end{pmatrix};
\begin{pmatrix}
A_{L,\text{out}} \\
A_{R,\text{out}}
\end{pmatrix}
= S_x
\begin{pmatrix}
A_{L,\text{in}} \\
A_{R,\text{in}}
\end{pmatrix},
S_x = \frac{1}{q} \begin{pmatrix} p^* & 1 \\ 1 & -p \end{pmatrix}
$$

(4)

It is assumed that the amplitudes $A_{L,\text{in}}(k)$ and $A_{R,\text{in}}(k)$ are independent and equal to zero for $k \leq 0$ as well as obey the condition $|A_{L,\text{in}}(k)|^2 + |A_{R,\text{in}}(k)|^2 = 1$. When changing the sign of the wave number $k$, the incoming and outgoing waves change roles: $A_{L,\text{in}}(-k) \equiv A_{L,\text{out}}(k)$, $A_{R,\text{in}}(-k) \equiv A_{R,\text{out}}(k)$, and $A_{L,\text{out}}(-k) \equiv A_{L,\text{in}}(k)$, $A_{R,\text{out}}(-k) \equiv A_{R,\text{in}}(k)$. The primed variables are linked by the relations (3).

Our next step is to determine the spaces of in and out asymptotes – freely moving wave packets that describe non-stationary localized (physical) states of a particle in the limits $t \to -\infty$ and $t \to +\infty$, respectively (that is, at the initial and final stages of scattering).

3 The space of in and out asymptotes in the formalism of the scattering matrix

Note, in the general case the in asymptote has two components. That is, it represents a superposition of the left and right asymptotes moving toward the barrier in the region $(a, \infty)$, in the general case the in asymptote has two components. That is, it represents a superposition of the left and right asymptotes moving toward the barrier in the region $(−\infty, −a)$ and $(a, \infty)$, respectively. The same concerns the out asymptote, but its left and right asymptotes move away from the barrier.

Let $A_{L,\text{out}}$ and $A_{R,\text{in}}$ be the amplitudes of waves that move, on the OX-axis, from the right to the left. Then

$$
\Psi_{L,\text{in}}(k, t) = A_{L,\text{in}}(k)e^{-iE(k)t/\hbar}, \quad \Psi_{R,\text{in}}(k, t) = A_{R,\text{in}}(-k)e^{-iE(k)t/\hbar}
$$

be wave packets moving toward the barrier in the remote regions $A$ and $B$ that lie in the intervals $(-\infty, -a)$ and $(a, \infty)$, respectively; and

$$
\Psi_{L,\text{out}}(k, t) = A_{L,\text{out}}(-k)e^{-iE(k)t/\hbar}, \quad \Psi_{R,\text{out}}(k, t) = A_{R,\text{out}}(k)e^{-iE(k)t/\hbar}
$$

be wave packets moving away from the barrier in the regions $A$ and $B$, respectively.

According to the item (a), in the limits $t \to \pm \infty$, the left and right components of in and out asymptotes are nonzero, in the x-space, within the nonoverlapping intervals $(-\infty, -a)$ and $(a, \infty)$. This means that in these limiting cases the space $\mathcal{H}_\text{as}$ represents a direct sum of the subspaces $\mathcal{H}_L$ and $\mathcal{H}_R$ of left and right asymptotes, respectively: $\mathcal{H} = \mathcal{H}_\text{as} = \mathcal{H}_L \oplus \mathcal{H}_R$. And, if this is so in the x-representation, this must also be valid in the $k$-representation. The item (a) also implies that the left and right asymptotes are well localized, both in the x- and k-spaces: they are such that the average values of the operators $\hat{X}^n$ and $\hat{P}^n$ exist for any value of $n$; here $\hat{X}$ and $\hat{P}$ are the position and momentum operators, respectively.

To construct asymptotes with such properties in the k-space, we will assume that the functions $A_{L,\text{in}}(k)$ and $A_{R,\text{in}}(k)$ belong to the spaces $S(\Omega^+_k)$ and $S(\Omega^-_k)$, respectively; where $S(\Omega^+_k)$ is the Schwartz subspace of infinitely differentiable functions which are zero on the semiaxis $(-\infty, 0]$ and diminish in the limit $k \to -\infty$ more rapidly than any power function; $S(\Omega^-_k)$ is the Schwartz subspace of infinitely differentiable functions which are zero on the semiaxis $[0, +\infty)$ and diminish in the limit $k \to +\infty$ more rapidly than any power function. Thus, the wave packets $\Psi_{L,\text{in}}(k, t)$ and $\Psi_{R,\text{in}}(k, t)$ belong to the subspace $S(\Omega^+_k)$, while $\Psi_{L,\text{out}}(k, t)$ and $\Psi_{R,\text{out}}(k, t)$ belong to the subspace $S(\Omega^-_k)$.

And, as a consequence, in the $k$-representation, the space $\mathcal{H}$, in the limits $t \to \pm \infty$, represents the sum of the non-overlapping subspaces $S(\Omega^+_k)$ and $S(\Omega^-_k)$: $\mathcal{H} = \mathcal{H}_\text{as} = S(\Omega^+_k) \oplus S(\Omega^-_k)$.

However, we have also to take into account that the left and right asymptotes from these two $k$-subspaces must be such that their Fourier images are localized, in the x-space, in the remote non-overlapping spatial regions $A$ and $B$. In order to ensure this property for both stages of scattering,
it is sufficient to construct the space of in asymptotes with such a property (the corresponding out asymptotes can be found with making use of the scattering matrix).

Let \( A_{+}(k) \) and \( A_{-}(k) \) be such wave packets from \( S(\Omega_{L}^{+}) \) and \( S(\Omega_{L}^{-}) \), respectively, that their "centers of mass" (CMs) are positioned at the origin of coordinates. Then the needed left and right in asymptotes, in the k-representation, can be written as \( A_{L,in}(k) = A_{+}(k)e^{ikD} \) and \( A_{R,in}(k) = A_{-}(k)e^{-ikD} \), respectively; here \( D \) is the distance between the CM of each wave packet and the origin of coordinates. For example, we can take as the left and right in asymptotes the following two wave functions: \( A_{L,in}(k) = N \cdot \exp \left[ \frac{-(k-k_{0})^{2}}{2} + ikD \right] \) for \( k \in (0, \infty) \) and \( A_{R,in}(k) = N \cdot \exp \left[ \frac{(k+k_{0})^{2}}{2} - ikD \right] \) for \( k \in (-\infty, 0) \); here \( N \) is the normalization constant, \( k_{0} \) and \( l \) are positive parameters. To ensure the localization of the left and right in asymptotes in the remote spatial regions \( \mathcal{A} \) and \( \mathcal{B} \), respectively, we have to consider these expressions in the limit \( D \to \infty \).

So, the in asymptotes \( \Psi_{L,in} \) and \( \Psi_{R,in} \), as well as the corresponding out asymptotes \( \Psi_{L,out} \) and \( \Psi_{R,out} \) do not overlap each other both in the \( k \)-space and in the \( x \)-space:

\[
\Psi_{L,in}(k,t), \Psi_{R,out}(k,t) \in S(\Omega_{L}^{+}) ,\quad \Psi_{R,in}(k,t), \Psi_{L,out}(k,t) \in S(\Omega_{L}^{-}), \\
\Psi_{R,in}(x,t), \Psi_{R,out}(x,t) \in S(\Omega_{L}^{+}) ,\quad \Psi_{L,in}(x,t), \Psi_{L,out}(x,t) \in S(\Omega_{L}^{-}).
\]

4 On the rigged (equipped) Hilbert space associated with the process

Note that in a more accurate description of state spaces in quantum mechanics (see, e.g., [6–8]) the spaces of antilinear functionals over \( \Phi \), which includes right eigenvectors of one-particle operators \( \hat{X} \) and \( \hat{P} \) (the corresponding bra-vectors belong to the space \( \Phi' \) of linear functionals over \( \Phi \)). The term "physical states" implies that for such states expectation values exist for any finite degree of the operators \( \hat{X} \) and \( \hat{P} \). According to [6–8], such states belong to the Schwartz space \( S \) which is invariant with respect to the Fourier-transform.

The space of asymptotes should be denoted now as \( \Phi_{as} \), and namely \( \Phi_{as} \) spans the whole space \( \Phi \) when there are no bound states. That is, now the space \( \Phi \) has (together with \( \Phi_{as} \)) a nontrivial structure in the limits \( t \to \pm \infty \). If one considers asymptotes in the k-representation, \( \Phi_{as} = \Phi_{as}(\Omega_{L}^{+}) \oplus \Phi_{as}(\Omega_{L}^{-}) \) where \( \Phi_{as}(\Omega_{L}^{+}) = S(\Omega_{L}^{+}) \) and \( \Phi_{as}(\Omega_{L}^{-}) = S(\Omega_{L}^{-}) \). While in the x-representation \( \Phi_{as} = \Phi_{as}(\Omega_{L}^{+}) \oplus \Phi_{as}(\Omega_{L}^{-}) \) where \( \Phi_{as}(\Omega_{L}^{+}) = S(\Omega_{L}^{+}) \) and \( \Phi_{as}(\Omega_{L}^{-}) = S(\Omega_{L}^{-}) \). Thus, there are reasons to believe that the space \( H^{rig} \) has, too, a more complex structure than it was assumed in [6–8].

5 Asymptotic states as two-component wave functions

Since the left and right components of the in asymptote \( |\Psi_{in}\rangle = |\Psi_{L,in}\rangle + |\Psi_{R,in}\rangle \) (in the limit \( t \to -\infty \)) and out asymptote \( |\Psi_{out}\rangle = |\Psi_{L,out}\rangle + |\Psi_{R,out}\rangle \) (in the limit \( t \to +\infty \)) belong to the non-overlapping spaces, their scalar products equal to zero and the expressions for the norms of the vectors \(|\Psi_{in}\rangle\) and \(|\Psi_{out}\rangle\) do not contain interference terms. That is, \( \langle \Psi_{in}|\Psi_{in}\rangle = \langle \Psi_{L,in}|\Psi_{L,in}\rangle + \langle \Psi_{R,in}|\Psi_{R,in}\rangle = 1 \) and \( \langle \Psi_{out}|\Psi_{out}\rangle = \langle \Psi_{L,out}|\Psi_{L,out}\rangle + \langle \Psi_{R,out}|\Psi_{R,out}\rangle = 1 \).

The scattering matrix formalism prompts us that the two-component in and out asymptotes can be presented, similarly to the Pauli spinor, in the form of two-component columns. Thus, we will believe further that any two asymptotes \(|\chi\rangle\) and \(|\psi\rangle\) can be written as \( \begin{pmatrix} \chi_{1} \\ \chi_{2} \end{pmatrix} \) and \( \begin{pmatrix} \psi_{1} \\ \psi_{2} \end{pmatrix} \), respectively, and their norms and scalar products are defined as \( \langle \chi|\chi\rangle = \langle \chi_{1}|\chi_{1}\rangle + \langle \chi_{2}|\chi_{2}\rangle \), \( \langle \psi|\psi\rangle = \langle \psi_{1}|\psi_{1}\rangle + \langle \psi_{2}|\psi_{2}\rangle \), \( \langle \chi|\psi\rangle = \langle \chi_{1}|\psi_{1}\rangle + \langle \chi_{2}|\psi_{2}\rangle \).

Note, the conformity between the components of any asymptote and the corresponding column depends on the scattering matrix taken as the basis for the transition to the "two-column representation". In the \( k \)-space we have to use the formalism of the scattering matrix \( S_{k} \), while in the \( x \)-space we have to use the formalism of the scattering matrix \( S_{x} \). And of importance is to stress that we can use either the \( k \)-representation or the \( x \)-representation!
5.1 $k$-representation

Note that the matrix $S_k$ acts in the space of columns whose first elements describe waves moving along the $OX$-axis from the left to the right, while the second elements describe waves moving in the opposite direction. In other words, the first elements of such columns are wave functions that belong to the subspace $S(O_k^+)$, while the second elements are wave functions from $S(O_k^-)$. Thus, these asymptotes can be presented in the form $|\Psi_{in}\rangle = \begin{pmatrix} \Psi_{L,in} \\ \Psi_{R,in} \end{pmatrix}$, $|\Psi_{out}\rangle = \begin{pmatrix} \Psi_{R,out} \\ \Psi_{L,out} \end{pmatrix}$. The corresponding bra-vectors represent rows: $\langle \Psi_{in} | = \begin{pmatrix} \Psi_{L,in}^* \\ \Psi_{R,in}^* \end{pmatrix}$, $\langle \Psi_{out} | = \begin{pmatrix} \Psi_{R,out}^* \\ \Psi_{L,out}^* \end{pmatrix}$.

Let us consider such a pair of vectors $|\phi^{(1)}_{k'}\rangle$ and $|\phi^{(2)}_{k'}\rangle$ with the parameter $k' > 0$, as well as a pair of vectors $|\phi^{(1)}_{k''}\rangle$ and $|\phi^{(2)}_{k''}\rangle$ with a given parameter $x' (|x'| > a)$, that

$$
\phi^{(1)}_{k'}(k) = \begin{pmatrix} \delta(k-k') \\ 0 \end{pmatrix}, \quad \phi^{(2)}_{k'}(k) = \begin{pmatrix} 0 \\ \delta(k+k') \end{pmatrix}; \quad \phi^{(1)}_{k''}(k) = \begin{pmatrix} e^{ikx'} \\ 0 \end{pmatrix}, \quad \phi^{(2)}_{k''}(k) = \begin{pmatrix} 0 \\ e^{-ikx'} \end{pmatrix}.
$$

The first pair among them gives the eigenvectors of the operator $\hat{P}$; with $\hat{P}|\phi^{(1)}_{k'}\rangle = +\hbar k'|\phi^{(1)}_{k'}\rangle$, $\hat{P}|\phi^{(2)}_{k'}\rangle = -\hbar k'|\phi^{(2)}_{k'}\rangle$, and $\langle \phi^{(1)}_{k'} | \phi^{(2)}_{k'} \rangle = 0$. While the second pair gives the eigenvectors of the position operator $\hat{X} = i\hbar \frac{\partial}{\partial k}$; with $\hat{X}|\phi^{(1)}_{k''}\rangle = -x'|\phi^{(1)}_{k''}\rangle$, $\hat{X}|\phi^{(2)}_{k''}\rangle = +x'|\phi^{(2)}_{k''}\rangle$, and $\langle \phi^{(1)}_{k''} | \phi^{(2)}_{k''} \rangle = 0$.

Note that, in the $k$-representation, the eigenvectors $|\phi^{(1)}_{k'}\rangle$ and $|\phi^{(2)}_{k'}\rangle$ of the momentum operator, corresponding to its different eigenvalues, belong also to the different sectors $S(O_k^+)$ and $S(O_k^-)$. While, for example, the eigenvectors $|\phi^{(1)}_{k''}\rangle$ and $|\phi^{(2)}_{k''}\rangle$, corresponding to the different eigenvalues of the position operator, belong to the same sector $S(O_k^0)$.

The stationary in and out asymptotes with a given positive value $k'$ can be written now in the form $\Psi_{in}(k,k') = A_{L,in}(k)|\phi^{(1)}_{k'}(k) + A_{R,in}(-k)|\phi^{(2)}_{k'}(k) \rangle$ and $\Psi_{out}(k,k') = A_{R,out}(k)|\phi^{(1)}_{k'}(k) + A_{L,out}(-k)|\phi^{(2)}_{k'}(k) \rangle$.

5.2 $x$-representation

In the $x$-representation we use the matrix $S_x$, because now $|\Psi_{in}\rangle = \begin{pmatrix} \Psi_{L,in} \\ \Psi_{R,in} \end{pmatrix}$ and $|\Psi_{out}\rangle = \begin{pmatrix} \Psi_{L,out} \\ \Psi_{R,out} \end{pmatrix}$.

That is, $S_x$ acts in the space of columns whose first elements describe waves that constitute wave packets moving in the spatial region $x < -a$, while their second elements describe waves that constitute wave packets moving in the region $x > +a$. Now, the first elements of columns are functions from the subspace $S(O_x^-)$, while the second elements are functions from the subspace $S(O_x^+)$.

Let us consider such a pair of vectors $|\chi^{(1)}_{k'}\rangle$ and $|\chi^{(2)}_{k'}\rangle$ with a given parameter $k'$, as well as such a pair of vectors $|\chi^{(1)}_{k''}\rangle$ and $|\chi^{(2)}_{k''}\rangle$ with the parameter $x' > 0$, that

$$
\chi^{(1)}_{k'}(x) = \begin{pmatrix} e^{ik'x} \\ 0 \end{pmatrix}, \quad \chi^{(2)}_{k'}(x) = \begin{pmatrix} 0 \\ e^{-ik'x} \end{pmatrix}; \quad \chi^{(1)}_{k''}(x) = \begin{pmatrix} \delta(x+x') \\ 0 \end{pmatrix}, \quad \chi^{(2)}_{k''}(x) = \begin{pmatrix} 0 \\ \delta(x-x') \end{pmatrix}.
$$

The first pair of vectors gives the eigenvectors of the operator $\hat{P} = -i\hbar \frac{\partial}{\partial x}$; with $\hat{P}|\chi^{(1)}_{k'}\rangle = +\hbar k'|\chi^{(1)}_{k'}\rangle$, $\hat{P}|\chi^{(2)}_{k'}\rangle = -\hbar k'|\chi^{(2)}_{k'}\rangle$, and $\langle \chi^{(1)}_{k'} | \chi^{(2)}_{k'} \rangle = 0$. While the second pair gives the eigenvectors of the position operator $\hat{X} = x$: we have $\hat{X}|\chi^{(1)}_{k''}\rangle = -x'|\chi^{(1)}_{k''}\rangle$, $\hat{X}|\chi^{(2)}_{k''}\rangle = +x'|\chi^{(2)}_{k''}\rangle$, and $\langle \chi^{(1)}_{k''} | \chi^{(2)}_{k''} \rangle = 0$.

Similarly, in the $x$-representation, the eigenvectors $\chi^{(1)}_{k'}(x)$ and $\chi^{(2)}_{k'}(x)$ of the position operator, corresponding to its different eigenvalues, belong to the different sectors $S(O_x^-)$ and $S(O_x^+)$). While, for example, the eigenvectors $|\phi^{(1)}_{k''}\rangle$ and $|\phi^{(2)}_{k''}\rangle$, corresponding to the different eigenvalues of the momentum operator, belong to the same sector $S(O_x^0)$.

The stationary in and out states for a given positive value $k$ can now be written in the form $\Psi_{in}(x;k) = A_{L,in}(k)|\chi^{(1)}_{k}(x) + A_{R,in}(k)|\chi^{(2)}_{k}(x)$ and $\Psi_{out}(x;k) = A_{L,out}(k)|\chi^{(1)}_{k}(x) + A_{R,out}(k)|\chi^{(2)}_{k}(x)$. 

6 The Pauli matrix $\sigma_3$ as a superselection operator in the space of asymptotes

6.1 $k$-representation

Note that the vectors $|\phi_k^{(1)}\rangle$, $|\phi_k^{(2)}\rangle$, $|\phi_{k'}^{(1)}\rangle$ and $|\phi_{k'}^{(2)}\rangle$ are also the eigenvectors of the Pauli matrix $\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. Indeed, $\sigma_3|\phi_k^{(1)}\rangle = |\phi_k^{(1)}\rangle$, $\sigma_3|\phi_k^{(2)}\rangle = -|\phi_k^{(2)}\rangle$; $\sigma_3|\phi_{k'}^{(1)}\rangle = |\phi_{k'}^{(1)}\rangle$, $\sigma_3|\phi_{k'}^{(2)}\rangle = -|\phi_{k'}^{(2)}\rangle$.

Thus, though $\hat{X}$ and $\hat{P}$ do not commute with each other, each of them commutes with the operator $\sigma_3$. It is also important to stress (see [9]) that the operator $\sigma_3$ can be expressed via the projection operators $P_+ = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$, $P_- = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$. Namely, $\sigma_3 = P_+ - P_-$.

Since the state space of a particle involved in the 1D scattering process is complete (see, e.g., [7]) (and no matter which stage of this process is regarded), the self-adjoint operator $\sigma_3$ can be treated (see [9,10]) as the superselection operator which divides the state space $\mathcal{H}_{as}^{rig}$, in the $k$-representation, into two coherent sectors ($\mathcal{H}_{as}^{rig}$ is the rigged Hilbert space $\mathcal{H}_{as}^{rig}$ in the limits $t \to \mp \infty$):

$$\mathcal{H}_{as}^{rig} = \mathcal{H}_{as}^{rig}(\Omega_1^+) \oplus \mathcal{H}_{as}^{rig}(\Omega_2^-);$$

$$\mathcal{H}_{as}^{rig}(\Omega_1^+) = \Phi_{as}(\Omega_1^+) \subset L^2_{as}(\Omega_1^+) \subset \Phi_{as}^x(\Omega_1^+), \quad \mathcal{H}_{as}^{rig}(\Omega_2^-) = \Phi_{as}(\Omega_2^-) \subset L^2_{as}(\Omega_2^-) \subset \Phi_{as}^x(\Omega_2^-).$$

Here the subspace $\mathcal{H}_{as}^{rig}(\Omega_1^+)$ represents the coherent sector (let’s call it the ‘top coherent sector’) that corresponds to the eigenvalue $+1$ of the operator $\sigma_3$, while the subspace $\mathcal{H}_{as}^{rig}(\Omega_2^-)$ is the ‘lower coherent sector’ corresponding to the eigenvalue $-1$. It is evident that $|\phi_{k'}^{(1)}\rangle$, $|\phi_{k'}^{(2)}\rangle \in \Phi_{as}^x(\Omega_1^+)$, and $|\phi_k^{(1)}\rangle$, $|\phi_k^{(2)}\rangle \in \Phi_{as}^x(\Omega_2^-)$.

6.2 $x$-representation

Now the vectors $|\chi_k^{(1)}\rangle$, $|\chi_k^{(2)}\rangle$, $|\chi_{k'}^{(1)}\rangle$ and $|\chi_{k'}^{(2)}\rangle$ are eigenvectors of the matrix $\sigma_3$:

$$\sigma_3|\chi_k^{(1)}\rangle = |\chi_k^{(1)}\rangle, \quad \sigma_3|\chi_k^{(2)}\rangle = -|\chi_k^{(2)}\rangle; \quad \sigma_3|\chi_{k'}^{(1)}\rangle = |\chi_{k'}^{(1)}\rangle, \quad \sigma_3|\chi_{k'}^{(2)}\rangle = -|\chi_{k'}^{(2)}\rangle.$$

That is, as is expected, two coherent sector arise. In the $x$-representation,

$$\mathcal{H}_{as}^{rig} = \mathcal{H}_{as}^{rig}(\Omega_x^-) \oplus \mathcal{H}_{as}^{rig}(\Omega_x^+);$$

$$\mathcal{H}_{as}^{rig}(\Omega_x^-) = \Phi_{as}(\Omega_x^-) \subset L^2_{as}(\Omega_x^-) \subset \Phi_{as}^x(\Omega_x^-), \quad \mathcal{H}_{as}^{rig}(\Omega_x^+) = \Phi_{as}(\Omega_x^+) \subset L^2_{as}(\Omega_x^+) \subset \Phi_{as}^x(\Omega_x^+).$$

Now the eigenvalue $+1$ of the superselection operator $\sigma_3$ is associated with functions of the subspace $\mathcal{H}_{as}^{rig}(\Omega_x^-)$ (let’s call it the ‘left coherent sector’, while the eigenvalue $-1$ is associated with functions that belong to the subspace $\mathcal{H}_{as}^{rig}(\Omega_x^+)$ (let’s call it the ‘right coherent sector’). It is evident that $|\chi_k^{(1)}\rangle$, $|\chi_k^{(2)}\rangle \in \Phi_{as}^x(\Omega_x^-)$ and $|\chi_{k'}^{(1)}\rangle$, $|\chi_{k'}^{(2)}\rangle \in \Phi_{as}^x(\Omega_x^+)$.}

7 Superselection rule and superposition principle for the scattering process

According to the theory of SSRs [9,10], any superposition of pure states from the same coherent sector gives another pure state in this sector, while any superposition of pure states from different coherent sectors represents a mixed state. Thus, any superposition of states from the coherent sectors $\Phi_{as}(\Omega_x^-)$ and $\Phi_{as}(\Omega_x^+)$, in the $x$-representation (or from the coherent sectors $\Phi_{as}(\Omega_1^+)$ and $\Phi_{as}(\Omega_2^-)$, in the $k$-representation) represents a mixed state. Born’s interpretation of pure states is inapplicable to such a superposition – its squared modulus cannot be treated as the probability distribution in the $x$-space (or in the $k$-space), and the average value of any observable can not be defined for such a superposition.
In the general case the scattering matrices (4) do not commute with the superselection operator $S$. The unilateral scattering as a process of conversion of a pure state into a mixed one considered as a "mixture" of two subprocesses, each representing the unilateral scattering.

Thus, at the initial stage of scattering the phases $\lambda$ and $\nu$ are real phases. Then

$$\langle \psi_\lambda | \hat{O} | \psi_\lambda \rangle = \langle \psi_\nu | \hat{O} | \psi_\nu \rangle = \langle \hat{O} | \hat{O} | \psi_\lambda \rangle + \langle \psi_\lambda | \hat{O} | \psi_\nu \rangle.$$

This means that in the general case the Shrödinger dynamics crosses the superselection sectors of the Hilbert space associated with this scattering process.

There are only two particular cases when one of these two scattering matrices commutes with $S$. Namely, this takes place when either reflection coefficient $R(k)$ or the transmission coefficient $T(k)$ is zero. In the first case, which is associated with the resonant transmission of a particle through the potential barrier, $[S, S_3] = 0$: in this case the coherent sectors $\Phi_{as}(\Omega_k^+)$ and $\Phi_{as}(\Omega_k^-)$ are invariant with respect to the Shrödinger dynamics. In the second case, which is associated with the full reflection of a particle off the ideally opaque potential barrier, $[S, S_3] = 0$: in this case the coherent sectors $\Phi_{as}(\Omega_k^+)$ and $\Phi_{as}(\Omega_k^-)$ remain invariant in the course of the scattering process.

Let us consider the general case for the unilateral one-dimensional scattering, when there is only one source of particles located, for example, to the left of the barrier, that is, in the region $A$. Now

$$\Psi_{in}(x, t) = \int_{-\infty}^{\infty} A_{L,in}(k) \chi_{k}^{(1)}(x) e^{-iE(k)t/\hbar} \, dk; \quad \Psi_{out}(x, t) = \Psi_{L,out}(x, t) + \Psi_{R,out}(x, t), \quad (7)$$

$$\Psi_{L,out} = \int_{-\infty}^{\infty} A_{L,in}(k) \frac{p_{x}(k)}{q(k)} \chi_{-k}^{(1)}(x) e^{-iE(k)t/\hbar} \, dk, \quad \Psi_{R,out} = \int_{-\infty}^{\infty} A_{L,in}(k) \frac{1}{q(k)} \chi_{k}^{(2)}(x) e^{-iE(k)t/\hbar} \, dk;$$

$$\langle \Psi_{in} | \Psi_{in} \rangle = \mathcal{T} + \mathcal{T} = 1 \text{ where } \mathcal{T} = \langle \Psi_{R,out} | \Psi_{R,out} \rangle, \quad \mathcal{T} = \langle \Psi_{L,out} | \Psi_{L,out} \rangle.$$
interpretation of pure states to such superpositions. Thus, the unilateral scattering like the bilateral scattering is a “mixture” of two alternative subprocesses, and a complete quantum model of this process must provide the way of tracing its (“pure”) subprocesses at all stages of scattering.

This model must take into account that the in and out asymptotes of each subprocess evolve within a single coherent sector, either in the \(x\) - or \(k\)-space. For example, for the process with the asymptotes \((\Omega, \pm x)\), the in and out asymptotes of the transmission subprocess evolve in a single coherent sector \(\Phi_{\text{as}}(\Omega^+_k)\) in the \(k\)-space, while those of the reflection subprocess evolve within a single coherent sector \(\Phi_{\text{as}}(\Omega^-_k)\) in the \(x\)-space. At the same time the in and out asymptotes of the transmission subprocess lie in the different coherent sectors \(\Phi_{\text{as}}(\Omega^+_x)\) and \(\Phi_{\text{as}}(\Omega^-_x)\) in the \(x\)-space, and those of the reflection subprocess lie in the different coherent sectors \(\Phi_{\text{as}}(\Omega^+_k)\) and \(\Phi_{\text{as}}(\Omega^-_k)\) in the \(k\)-space.

9 Conclusion

It is shown that in a quantum description of scattering a nonrelativistic particle on a one-dimensional potential barrier the unboundedness of the position operator plays a crucial role and, as a consequence, the well-known Stone-von Neumann theorem is inapplicable to this process – the Schrödinger representation associated with this process is reducible. It is shown that there is a dichotomous-context-induced superselection rule with the Pauli matrix \(\sigma_3\) as a superselection operator. It divides the space of asymptotes, both in the coordinate and momentum representations, into the direct sum of two coherent sectors. Of importance is the fact that the matrix \(\sigma_3\) does not commute with the scattering matrix, what means that the Schrödinger dynamics crosses the coherent sectors in the course of the unilateral one-dimensional scattering – the initial pure state is converted into a final mixed state. The quantum mechanical formalism developed for pure states can be applied only to the subprocesses of this scattering process (transmission and reflection).

References

1. Reed, M. and Simon, B.: Methods of modern mathematical physics. III: Scattering theory. Academic Press, Inc., (1979)
2. Prugovečki, E.: Quantum mechanics in Hilbert space. Academic Press. New York and London, (1971)
3. Taylor, J.R.: Scattering theory. The quantum theory of nonrelativistic collisions. John Wiley and Sons, (1972)
4. Hall, B.C.: Quantum theory for mathematicians. Springer, (2013)
5. Chuprikov, N.L.: Transfer matrix of a one-dimensional Schrödinger equation. Sov. Semicond. 26, 2040–2047 (1992)
6. de la Madrid, R.: The rigged Hilbert space of the algebra of the one-dimensional rectangular barrier potential. J. Phys. A: Math. Gen. 37, 8129–8157 (2004)
7. Sushko, V.N., Khoruzhii, S.S.: Vector states on algebras of observables and superselection rules. Theoretical and Mathematical Physics. 4, 877–889 (1970)
8. Horuzhy, S.S.: Superposition principle in Algebraic quantum theory. Theoretical and Mathematical Physics. 23, 413–421 (1975)
9. Sushko, V.N., Khoruzhii, S.S.: Vector states on algebras of observables and superselection rules I. Vector states and Hilbert space. Theoretical and Mathematical Physics. 4, 758–774 (1970)
10. James, L.P. and Band, W.: Mutually Exclusive and Exhaustive Quantum States. Foundations of Physics, 6, No.2, 157–172 (1976)
11. Gilmore, T.Jr. and Park, J.: Superselection Rules in Quantum Theory: Part I. A New Proposal for State Restriction Violation. Foundations of Physics, 9, Nos. 7/8, 537–556 (1979)
12. Gilmore, T.Jr., and Park, J.: Superselection Rules in Quantum Theory: Part II. Subensemble Selection. Foundations of Physics, 9, Nos. 10, 739–749 (1979)
13. Earman, J.: Superselection Rules for Philosophers. Erkenntnis. 69, 377–414 (2008)
14. Khrennikov, A.Yu.: The principle of supplementarity: a contextual probabilistic viewpoint to complementarity, the interference of probabilities and incompatibility of variables in quantum mechanics. Found. Phys. 35(10), 1655–1693 (2005)
15. Accardi, L.: The probabilistic roots of the quantum mechanical paradoxes. Diner S. et al. (eds.) The Wave-Particle Dualism: A Tribute to Louis de Broglie on his 90th Birthday, 297–330 (1984)