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COEXISTENCE OF A BOUND STATE AND SCATTERING AT THE SAME ENERGY VALUE: A QUANTUM PARADOX

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There is no paradox if we separate a finite range space area by an unpenetrable potential barrier and get (parallel) spectral branches: a discrete one for bound states inside the trap and a continuum spectrum of scattering states outside the barrier.

Here the regions of bound and scattering states have no overlap and the trapped and propagating waves reside in different regions influenced by different parts of the external field.

But we shall show that some interactions can admit both confinement and scattering at the same energy value even without a strict space separation of propagating and bound waves.

In recent time the qualitative theory of constructing quantum systems with given properties has been developed (see [1, 3] and references therein) for the one-dimensional Schrödinger equation. The exactly solvable models of the inverse problem and supersymmetry (SUSY), see e.g.[4,7-11], provide us with algorithms of constructing quantum systems having any given spectral, scattering and decay characteristics. This gives one the possibility to convert quantum systems of a different nature into one another making our understanding of basic aspects of the quantum theory deeper. Physically clear rules of a complete set of potential transformations and their elementary constituents have been revealed by the computer visualization. This allows one to anticipate without calculations the main shape details of the potential having the prescribed features [1, 3]. We have found some curious unexpected effects among which are the ones described below.

The real objects have mainly a complex structure. In this case the multichannel wave equations are a powerful and universal tool of their description. This approach is a core of the unified theory of quantum reactions [12] and its generalization to processes with rearrangement of particles (see [5, 3] and references therein).

This method reduces the multi-dimensional Schrödinger equation in partial derivatives to the comparatively simple system of



coupled one-dimensional Schrödinger equations

$$-\psi_i''(x) + \sum_j V_{ij}(x)\psi_j(x) = E_i\psi_i(x)$$
(1)

where $V_{ij}(x)$ are the elements of the interaction matrix, $\psi_i(x)$ are the partial channel components of the wave function in the vector representation, $E_i = E - \epsilon_i$ are the partial channel energy values with the threshold energies ϵ_i above which the corresponding channels become open.

We shall also use matrix solutions of (1) where the first index means the channel number (i.e. partial equation number in (1)), the second one stands for the vector-column number in the matrix $\hat{\Psi}$ and designates the type of a boundary condition at x = 0. In what follows the hat stands for the matrix (including the vectorcolumn) or operator.

The qualitative arguments to resolve the "paradox" of coexistence of bound and scattering states may be the following. In the M-channel case there exist M linearly independent solutions of (1) for the same energy point vanishing at the origin. Above all thresholds these solutions are scattering states. The inverse problem and SUSY approach allow one to transform some of the scattering states into bound ones. If we transform one scattering state into a bound state embedded into the continuum at $E = E_b > \epsilon_i$; i = 1, 2, ...M), there will remain M - 1 scattering state solutions. As corresponding mathematical support we shall use the matrix generalization of the double SUSY transformation instead of the equivalent single one in the inverse problem approach. But by the SUSY-way we shall reveal another unexpected multichannel peculiarity, the absolutely transparent interaction matrix without bound states which has no analogues in the one-channel case.

Let \hat{H}_{-} be an initial matrix Hamiltonian of the multichannel system on the whole line which is described by the Schrödinger equation (1). Namely, (1) can be represented in a symbolical form $\hat{H}_{-}\hat{\psi} = E\hat{\psi}$ (the threshold energies ϵ_i can be included in \hat{H}_{-}). We shall consider the case of two channels. Let the threshold energies ϵ_i be different. We present this Hamiltonian, a second order differential operator, in the factorized form through differential first order operators [2]1997

$$\hat{H}_{-} = \hat{A}^{+}\hat{A}^{-} + \mathcal{E}, \qquad (2)$$

where \mathcal{E} is the factorization energy,

$$\hat{A}^{-} = -\frac{d}{dx} + \hat{W}(x) \tag{3}$$

and $\hat{A}^+ = \frac{d}{dx} + \{\hat{W}(x)\}^{\dagger}$ is Hermitian conjugation of \hat{A}^- . Here $\hat{W}(x)$ must be self-adjoint otherwise the Hamiltonian will include the undesired operator of the first derivative

$$\hat{H}_{-} = \hat{A}^{+}\hat{A}^{-} + \mathcal{E} = \left(\frac{d}{dx} + \{\hat{W}(x)\}^{\dagger}\right)\left(-\frac{d}{dx} + \hat{W}(x)\right) + \mathcal{E} = -\frac{d^{2}}{dx^{2}} + \hat{W}'(x) + \hat{W}(x)\frac{d}{dx} - \{\hat{W}(x)\}^{\dagger}\frac{d}{dx} + \{\hat{W}(x)\}^{\dagger}\hat{W}(x) + \mathcal{E}.$$

Let $\hat{\Psi}_{-}(x)$ be real matrix-valued solution of the equation (1) corresponding to the initial Hamiltonian \hat{H}_{-} at the energy $E = \mathcal{E}$ (i.e. $\hat{H}_{-}\hat{\Psi}_{-} = \mathcal{E}\hat{\Psi}_{-}$).

We can readily obtain $\hat{W}(x)$ from the equation

$$\hat{A}^-\hat{\Psi}_-(x) = 0 \tag{4}$$

which becomes an identity if we act on it by operator \hat{A}^+ . From (4) and (3) follows

$$\hat{W}(x) = \hat{\Psi}'_{-}(x)\hat{\Psi}_{-}(x)^{-1}.$$
(5)

In SUSY approach we get by permutting operators \hat{A}^{\pm} in (2) the transformed Hamiltonian $\hat{H}_{+} = \hat{A}^{-}\hat{A}^{+} + \varepsilon$ with the following expression for the transformed potential

$$\hat{V}_{+}(x) = \hat{V}_{-}(x) - 2\hat{W}'(x).$$
(6)

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The expression of the solutions for the transformed potential (6) at any energy value $E \neq \mathcal{E}$ is

$$\hat{\Psi}_{+}(x,E) = (-\frac{d}{dx} + \hat{W}(x))\hat{\Psi}_{-}(x,E)$$
(7)

where $\hat{\Psi}_{-}(x, E)$ is the solution for the initial potential. At the energy \mathcal{E} solutions of (1) with transformed potential \hat{V}_{+} can be found in the following way. Differential matrix Schrödinger equation of the second order at energy \mathcal{E} with the transformed potential (6) has two linearly independent matrix solutions (four vector solutions). We shall find them by solving two more simple first order differential equations:

$$\hat{A}^+ \hat{\Psi}_+(x,\mathcal{E}) = 0, \tag{8}$$

$$\hat{A}^{+}\hat{\Psi}_{+}(x,\mathcal{E}) = \hat{\Psi}_{-}(x).$$
 (9)

Indeed, designating by $\hat{\Upsilon}$ solutions of (8) and (9) and acting on both sides of these equations by the operator \hat{A}^- we get $\hat{A}^-\hat{A}^+\hat{\Upsilon} =$ $(\hat{H}_+ - \mathcal{E})\hat{\Upsilon} = 0$, which means that the Schrödinger equation is satisfied. These equations give two matrix linearly independent solutions

$$\hat{\Psi}_{+}(x,\mathcal{E}) = \{\hat{\Psi}_{-}(x)^{-1}\}^{T};$$
(10)

$$\hat{\tilde{\Psi}}_{+}(x,\mathcal{E}) = \{\hat{\Psi}_{-}(x)^{-1}\}^{T} \int_{0}^{x} \{\hat{\Psi}_{-}(y)\}^{T} \hat{\Psi}_{-}(y) dy.$$
(11)

Double SUSY formulae for $\hat{\Psi}$ and \hat{V} can be obtained using the same procedure as in the first step. The results coincide with the inverse problem ones. At the second step as an initial solution we take a combination of the first step matrix solutions $\hat{\Psi}_{++}(x)$ which are the solutions of the Schrödinger equation with potential $\hat{V}_{+}(x)$:

$$\hat{\Psi}_{++}(x) = \{\hat{\Psi}_{-}(x)^{-1}\}^{T} + c\{\hat{\Psi}_{-}(x)^{-1}\}^{T} \int^{x} \{\hat{\Psi}_{-}(y)\}^{T} \hat{\Psi}_{-}(y) dy (12)$$

where c is an arbitrary constant. As a result we have the following expression for second step potential

$$\hat{V}(x) = \hat{V}_{+}(x) - 2\frac{d}{dx}\hat{\tilde{W}}(x) =$$

$$= \hat{V}_{-}(x) - 2\frac{d}{dx}(\hat{\Psi}_{-}'(x)\{\hat{\Psi}_{-}(x)\}^{-1} + \hat{\Psi}_{++}'(x)\{\hat{\Psi}_{++}(x)\}^{-1}) =$$

$$= \hat{V}_{-}(x) - 2\frac{d}{dx}(c \ \hat{\Psi}_{-}(x)\{1 + c\int^{x}_{-}[\hat{\Psi}_{-}(y)]^{T}\hat{\Psi}_{-}(y)dy\}^{-1}\hat{\Psi}_{-}(x)^{T})(13)$$

One can be convinced of the correctness of the above formulae by the direct substitution of solutions and interaction matrices into the multichannel Schrödinger equation (1).

Let us use the following initial solution $\hat{\Psi}_{-}(x)$ referred to zero intraction $\hat{V}_{-}(x) = 0$ on the half-exis to create a bound state embedded into the continuum at $E = E_b \equiv \mathcal{E} > \epsilon_i$:

$$\hat{\Psi}_{-}(x) = \begin{pmatrix} \frac{c_1}{\sqrt{ck_1}} \sin(k_1 x) & 0\\ \frac{c_2}{\sqrt{ck_2}} \sin(k_2 x) & 0 \end{pmatrix}$$
(14)

where $k_i = \sqrt{E_b - \epsilon_i}$.

This gives according to (13) the following expression for V_{ij} (the indeces of the matrix $\hat{V}(x)$ are written explicitly):

$$V_{ij}(x) = -2\frac{d}{dx}\frac{1}{k_ik_j}\frac{c_ic_j\sin(k_ix)\sin(k_jx)}{1 + \frac{c_1^2}{k_1^2}(\frac{x}{2} - \frac{\sin(2k_1x)}{4k_1}) + \frac{c_2^2}{k_2^2}(\frac{x}{2} - \frac{\sin(2k_2x)}{4k_2})}.$$
 (15)

Let us now write expression for the regular solutions $\Phi_{ij}(x)$ at the energy $E = E_b \ (\Phi_{ij}(x)|_{x=0} = 0; \frac{d}{dx} \Phi_{ij}(x)|_{x=0} = \delta_{ij})$:

$$\Phi_{ij}(x) = \frac{1}{k_i} \sin(k_i x) \delta_{ij} - \frac{1}{k_i k_j^2} \frac{c_i c_j \sin(k_j x) (\frac{x}{2} - \frac{\sin(2k_j x)}{4k_j})}{1 + \frac{c_1^2}{k_1^2} (\frac{x}{2} - \frac{\sin(2k_1 x)}{4k_1}) + \frac{c_2^2}{k_2^2} (\frac{x}{2} - \frac{\sin(2k_2 x)}{4k_2})}.$$
(16)

The meaning of parameters c_i will be clarified further.

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As $x \to \infty$ matrix of regular solutions (16) has the following asymptotic behavior

$$\Phi_{ij}(x) \to \frac{1}{k_i} \sin(k_i x) \delta_{ij} - \frac{c_i c_j \sin(k_i x)}{k_i k_j^2 (\frac{c_1^2}{k_1^2} + \frac{c_2^2}{k_2^2})} + O(\frac{1}{x}).$$
(17)

It can be seen from this expression that the vector-columns making up the matrix $\Phi_{ij}(x)$ become linearly dependent asymptotically. In other words there exists a proper linear combination of the columns of $\Phi_{ij}(x)$ which decreases as $\sim \frac{1}{x}$ when $x \to \infty$ at $E = E_b$. The coefficients c_i of such a combination $\Psi_{i\ bound}(x) \equiv$ $\sum_j c_j \Phi_{ij}(x)$ are just the components of spectral weight vector [5] $(\Psi_{i\ bound}(x)|_{x=0} = 0, [\Psi_{i\ bound}]'(x)|_{x=0} = c_i)$ of the normalizable bound state $\Psi_{i\ bound}(x)$ embedded into the continuum:

$$\int_0^\infty \sum_i [\Psi_{i\ bound}(y)]^2 dy = 1$$

. Other linearly independent solution behaves asymptotically as $\sim \sin(k_i x)$ according to (17), e.g. as an eigenphase scattering state at $E = E_b$ (with zero eigenphaseshift). This means effective transparency of the interaction matrix. It is also possible to continue symmetrically the interaction matrix from the half axis to the whole axis with corresponding smooth continuation of the bound and scattering wave functions.

Now we shall use the first SUSY transformation to construct a transparent system without bound states. For the whole axis and initial $\hat{V}_{-}(x) = 0$ (free motion) we can choose

$$\hat{\Psi}_{-}(x) = \begin{pmatrix} m_1 e^{-\kappa_1 x} & e^{\kappa_1 x} \\ m_2 e^{-\kappa_2 x} & -\frac{m_1 \kappa_1}{m_2 \kappa_2} e^{\kappa_2 x} \end{pmatrix}$$
(18)

where $\kappa_i = \sqrt{\epsilon_i - \mathcal{E}}$.

Such a choice gives Hermitian W:

$$\hat{W}_{11}(x) = \frac{m_2^2 \kappa_1 \kappa_2 exp[(\kappa_1 - \kappa_2)x] - m_1^2 \kappa_1^2 exp[(\kappa_2 - \kappa_1)x]}{m_1^2 \kappa_1 exp[(\kappa_2 - \kappa_1)x] + m_2^2 \kappa_2 exp[(\kappa_1 - \kappa_2)x]},$$

$$\hat{W}_{12}(x) = \hat{W}_{21}(x) = -\frac{2\kappa_1 m_1 \kappa_2 m_2}{m_1^2 \kappa_1 exp[(\kappa_2 - \kappa_1)x] + m_2^2 \kappa_2 exp[(\kappa_1 - \kappa_2)x]}$$

$$\hat{W}_{22}(x) = \frac{m_1^2 \kappa_1 \kappa_2 exp[(\kappa_2 - \kappa_1)x] - m_2^2 \kappa_2^2 exp[(\kappa_1 - \kappa_2)x]}{m_1^2 \kappa_1 exp[(\kappa_2 - \kappa_1)x] + m_2^2 \kappa_2 exp[(\kappa_1 - \kappa_2)x]}.$$
 (19)

With this expression we get via formula (6) the absolutely transparent interaction matrix shown in Fig.1.



Fig.1. The two-channel absolutely transparent potential matrix with $\mathcal{E} = -0.5, m_1 = 1, m_2 = .001$ without a bound state. The thresholds are $\epsilon_1 = 0, \epsilon_2 = 1$.

The solutions $\hat{\Psi}_+(x,\mathcal{E})$ and $\tilde{\Psi}_+(x,\mathcal{E})$ have the following asymptotic behavior

$$\hat{\Psi}_{+}(x,\mathcal{E}) \sim \begin{pmatrix} e^{(2\kappa_{2}-\kappa_{1})x} & e^{-\kappa_{1}x} \\ e^{\kappa_{2}x} & e^{(-2\kappa_{1}+\kappa_{2})x} \end{pmatrix}, \hat{\tilde{\Psi}}_{+}(x,\mathcal{E}) \sim \begin{pmatrix} e^{-\kappa_{1}x}x & e^{\kappa_{1}x} \\ e^{-\kappa_{2}x} & e^{\kappa_{2}x}x \end{pmatrix}$$

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when $x \to -\infty$,

$$\hat{\Psi}_{+}(x,\mathcal{E}) \sim \begin{pmatrix} e^{\kappa_{1}x} & e^{(\kappa_{1}-2\kappa_{2})x} \\ e^{(2\kappa_{1}-\kappa_{2})x} & e^{-\kappa_{2}x} \end{pmatrix}, \\ \hat{\tilde{\Psi}}_{+}(x,\mathcal{E}) \sim \begin{pmatrix} e^{-\kappa_{1}x} & e^{\kappa_{1}x} \\ e^{-\kappa_{2}x}x & e^{\kappa_{2}x} \end{pmatrix}$$

when $x \to \infty$.

One can see from these expressions that it is impossible to construct any linear combination of $\hat{\Psi}_+(x,\mathcal{E})$ and $\hat{\tilde{\Psi}}_+(x,\mathcal{E})$ which would decrease as $x \to \pm \infty$ and hence be normalizable. Thus SUSY transformation with the choice of $\hat{\Psi}(x)$ (18) (and \hat{W} in the form (19) does not create a bound state at factorization energy \mathcal{E} but leads to a non-trivial reflectionless potential matrix $\hat{V}_+(x)$ (6) having no bound states, see Fig.1.

This exact result can also be explained qualitatively as follows. In the one-channel case there are necessary bound states in the reflectionless (soliton-type) potentials. There cannot be repulsion to avoid reflection. But any purely attractive potential on the whole axis has a bound state (a widely known fact). And in the two-channel case there are more degrees of freedom. There is a potential barrier in the element of the matrix $V_{11}(x)$ in Fig.1 which compensates attraction in another channel to exclude the bound state. It is curious that the reflection from the barrier in the first channel is also necessary for the complete transparency. There is mutual cancellation of the waves reflected from the barrier with the backward waves coming from the second channel as a result of the channel coupling $V_{12}(x)$ and having the opposite phase as was discovered in [1]. It is interesting that the transparent interaction matrix in [1] differs from the one in Fig.3 only by an additional soliton-like well which bears the bound state.

In summary, we have found that in special cases the interchannel exchange of waves for spectral rate of partial channel components can be destructive at asymptotics which gives decreasing bound state tails of the wave functions. And for another rate of partial channel components the exact asymptotic cancellation of wave functions is violated and there can remain allowed wave propagation to infinity (scattering). There are also multichannel reflecionless interactions (on the whole axis) without bound states which have no one-channel analogues. Both the cases are instructive demonstration of multichannel peculiarities enriching our quantum intuition.

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Чабанов В.М., Захарьев Б.Н. Сосуществование связанного состояния и рассеяния при одной энергии: квантовый «парадокс»

Демонстрируется пример многоканальной системы, имеющей как связанное (не квазисвязанное!) состояние, так и рассеяние при том же значении энергии *E*. Специальный вид взаимодействия способен запирать волны вблизи начала координат и одновременно допускать рассеяние (и даже прозрачность) в фиксированной спектральной точке. Такие матрицы взаимодействия и волновые функции могут быть продолжены на всю ось.

Другой многоканальной особенностью, не имеющей одноканального аналога, является класс абсолютно прозрачных матриц взаимодействия без связанных состояний.

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Chabanov V.M., Zakhariev B.N. Coexistence of a Bound State and Scattering at the Same Energy Value: a Quantum Paradox

The example of a multi-channel system which possesses both bound (not quasibound!) and scattering states at the same energy value E is demonstrated. A special interaction has ability to confine waves near the origin and simultaneously admit scattering (even with transparency) at the fixed spectral point. These interaction matrices and wave functions can be continued to the whole axis.

As another multi-channel peculiarity having no one-channel analogues was found a class of absolutely transparent interaction matrices without bound states.

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