Scattering theory with localized non-Hermiticities

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Abstract

In the context of the recent interest in solvable models of scattering mediated by non-Hermitian Hamiltonians (cf. H. F. Jones, Phys. Rev. D 76, 125003 (2007)) we show that the well known variability of the ad hoc choice of the metric Θ which defines the physical Hilbert space of states can help us to clarify several apparent paradoxes. We argue that with a suitable Θ a fully plausible physical picture of the scattering can be recovered. Quantitatively, our new recipe is illustrated on an exactly solvable toy model.
1 Introduction

Whenever one considers the one-dimensional differential Schrödinger equation

\[ \left[ -\frac{d^2}{dx^2} + V(x) \right] \psi(x) = E \psi(x), \quad x \in (-\infty, \infty) \]  

(1)

in the scattering regime, i.e., with the boundary conditions describing the transmitted and reflected waves,

\[ \psi(x) = \begin{cases} 
  e^{i\kappa x} + C e^{-i\kappa x}, & x \ll -1, \\
  D e^{i\kappa x}, & x \gg 1 
\end{cases} \]  

(2)

one usually assumes that the flow of probability is conserved, \( |C|^2 + |D|^2 = 1 \).

Recently, Jones [1] pointed out that several serious conceptual difficulties can arise when certain current tacit assumptions (demanding, typically, the reality of the potential \( V(x) \)) are, tentatively, weakened. He also presented several persuasive arguments why one should try to weaken these assumptions.

Among the latter arguments, the most persuasive support of theoretical as well as conceptual innovations would certainly lie in the undeniable success of the recent, phenomenologically motivated transition to certain manifestly non-Hermitian Hamiltonians generating real and observable spectra of bound states [2]. The idea (well known to mathematicians [3]) found, recently, several interesting applications in nuclear physics [4] and in field theory [5].

Of course, there exists an obvious difference between the bound-state problem (for which wave functions \( \psi(x) \) are localized) and the scattering scenario (where all the waves remain non-negligible all along the whole real axis). Jones [1] even came to a rather sceptical conclusion that the preservation of a sensible probabilistic interpretation of a generic non-Hermitian model of scattering may be quite costly and difficult even when the tentative introduction of a suitable non-Hermiticity in the Hamiltonian itself remains restricted to a very small domain of \( x \). Similar observations have been also made in a few older scattering models where the violation of the rule \( |C|^2 + |D|^2 = 1 \) has been explained and interpreted as a phenomenologically acceptable manifestation of the presence of some “hidden” degrees of freedom in the model [6].
Being not satisfied by these “effective” theories the author of ref. [1] formulated a much more ambitious project where the physical picture of scattering would parallel the above-mentioned “fundamental” theory of bound states based on non-Hermitian Hamiltonians [4, 5]. Unfortunately, the quantitative results of ref. [1] were not too encouraging (cf. also their recent completion [7]). In essence, the sensible probabilistic interpretation of the models under consideration seemed to require that the above-mentioned standard boundary conditions should be modified to read

\[ \psi(x) = \begin{cases} 
  e^{ix} + Ce^{-ix}, & x \ll -1, \\
  De^{ix} + D'e^{-ix}, & x \gg 1.
\end{cases} \] (3)

Unfortunately, this formula contains a strongly counterintuitive “backwards-running” component proportional to \( D' \neq 0 \) in the scattered solution.

In what follows we intend to weaken the resulting skepticism. We shall start from the same basic theoretical premise and postulate that the effective theories of refs. [6] are in fact not too interesting since they just mimic the presence of certain unknown dynamical mechanisms admitting, i.a., an annihilation and/or creation during the scattering. In this sense, we intend to search now for a new quantitative support for the possible feasibility and consistency of the alternative fundamental approach where one tries to re-establish the conservation of the probability.

In section [2] we shall commence our considerations by a brief and compact review of the most relevant results of ref. [1]. We summarize there the overall philosophy of the fundamental theory where the input Hamiltonian \( H \) [say, of eq. (1)] is interpreted as a mere auxiliary operator. One assumes that with this auxiliary operator the formal calculations become exceptionally simple. At the same time, the “correct” physics is assumed to be defined, via an invertible map \( \Omega \), in terms of a certain “true” physical Hamiltonian

\[ h = \Omega H \Omega^{-1} \] (4)

which is expected to be prohibitively complicated. For illustration one can recollect the “true nuclear physics” of ref. [4] where \( h \) was a full-fledged Hamiltonian of an atomic nucleus while \( H \) has been constructed as its much more easily tractable map.
In all the similar scenarios, the similarity mapping $\Omega$ must be assumed non-unitary – otherwise, one would return to the mere traditional, Hermitian class of Hamiltonians. In order to suppress or circumvent the related, mostly purely technical obstacles we decided to employ our recent bound-state experience [8] and to restrict our attention to a fairly restricted class of the solvable illustrative dynamical models. They are introduced and described in section 3.

The manifestly non-perturbative character of our present class of models will enable us to make use of the flexibility of the mappings $\Omega$ and to draw several consequences from the exact solvability of our models. In section 4 we shall show how some of the apparently unavoidable paradoxes of ref. [1] can find their explanation and resolution. In particular, for our manifestly non-Hermitian set of specific Hamiltonian-representing operators $H \neq H^\dagger$ we shall demonstrate that they can be assigned a consistent and unitary physical interpretation of the scattering based on standard asymptotic boundary conditions (2).

In section 5 a compact summary of our present constructive arguments will be complemented by a few optimistic remarks concerning the possible future extension of the class of our present models of scattering towards some less schematic non-Hermitian Hamiltonians.

2 Scattering from complex potentials

The mathematical background of the fundamental models of scattering from localized non-Hermitian centers will be illustrated here on a set of solvable models. On this level we shall demonstrate that a very natural interpretation of this type of scattering is feasible. On an abstract phenomenological level we shall stress that in our present update of the extension of the scattering theory of ref. [1] a core of observational consistency should and can be sought in an at least partial, asymptotic survival of the observability of the coordinates.
2.1 Jones’ solvable example

For the majority of the real and smooth one-dimensional short-range potentials the description of the scattering is routine. One solves the ordinary differential Schrödinger equation under the standard asymptotic boundary conditions. For the complex $V(x)$s in (1), fundamental theory makes the scattering unitary via an appropriate adaptation of the metric $\Theta$ in the Hilbert space of states. Unfortunately, an unexpected and unpleasant consequence has been detected in [1] where the replacement of the standard asymptotic boundary conditions (2) by their fairly counterintuitive “amendment” (3) has been found necessary in principle. Fortunately, in a concrete illustration using the complex delta function toy potential of ref. [9],

$$V^{(Mostafazadeh)}(x) = 2\lambda(1 + i\varepsilon)\delta(x)$$

the contribution of the nonvanishing coefficient $D'$ to the flow of probabilities proved negligible [1]. Thus, in the leading-order approximation it was possible to return to the original boundary conditions (2).

After such an approximate confirmation of the internal consistency of the fundamental theory approach a careful perturbation analysis of scattering by potential (5) has been performed in [1] leading to the intermediate result

$$|C|^2 + |D|^2 = \left(1 - \frac{2\varepsilon q}{1 + \varepsilon^2 + q^2}\right)^{-1}, \quad q = \frac{\sqrt{E}}{\lambda}. \quad (6)$$

In the naive effective-theory interpretation of this formula the non-conservation of the flow of probability merely reflects the fact that the manifestly non-Hermitian Hamiltonian $H$ is merely an auxiliary operator defined in the “wrong” Hilbert space $\mathcal{H}^{(unphysical)}$. One has to employ the map $\Omega$ to move to another, unitarily non-equivalent “correct” Hilbert space $\mathcal{H}^{(physical)}$ where the “true” representant (4) of the Hamiltonian remains safely Hermitian [1].
2.2 Long-range non-localities induced by the short-range potential: a paradox

One of the most unpleasant formal features of physical metric \( \Theta = \Theta(H) \) \[10\] in the Hilbert space of states \( \mathcal{H}^{(\text{physical})} \) is that it is usually strongly non-local even if the original potential is local, \( V = V(x) \) (cf. also \[8\]). This implies that it is hardly feasible to perform any computations in \( \mathcal{H}^{(\text{physical})} \). In the purely auxiliary Hilbert space \( \mathcal{H}^{(\text{unphysical})} \) the computations are assumed much easier. All the ket vectors \( |\psi\rangle \) which lie in the latter space lack, unfortunately, any direct physical interpretation. Even the standard requirement of the observability of the Hamiltonian degenerates, in this auxiliary space, to the identity \[11\]

\[ H^\dagger = \Theta H \Theta^{-1}. \] (7)

This relation represents the Hermiticity of the Hamiltonian \( h \) in \( \mathcal{H}^{(\text{physical})} \),

\[ h = \Omega H \Omega^{-1} = h^\dagger = \left(\Omega^{-1}\right)^\dagger H^\dagger \Omega^\dagger. \]

We may deduce that one has to put \( \Theta \equiv \Omega^\dagger \Omega \). In the language of mathematics we must guarantee that the physical metric \( \Theta \) is compatible with relations (7). Vice versa, any operator \( \sigma = \sigma^\dagger \) representing an observable in \( \mathcal{H}^{(\text{physical})} \) has to have its appropriate quasi-Hermitian partner \( \Sigma \) in \( \mathcal{H}^{(\text{unphysical})} \) which obeys an analogue of eq. (7) using the same metric \[12\].

The shift \( \varepsilon \) in eq. \[5\] has been assumed small in ref. \[1\]. This opened the possibility of an explicit use of Mostafazadeh’s metric \[9\] available in perturbation-series form

\[ \Theta^{(\text{Mostafazadeh})} \equiv \eta = I + \varepsilon \eta^{(1)} + \mathcal{O}(\varepsilon^2). \] (8)

In coordinate representation the unit operator \( I \) becomes represented by the delta-function kernel \( \delta(x - y) \) but a manifest and large nonlocality emerges already in the first perturbation order,

\[ \eta^{(1)}(x, y) = \frac{\lambda}{2} \text{sgn} (y^2 - x^2) \left[ \theta(xy) e^{-\lambda|x-y|} + \theta(-xy) e^{-\lambda|x+y|} \right]. \] (9)

The emergence of such a nonlocality leads to serious problems because “the physical picture of the scattering is completely changed” since, on the positive half-axis the
physical wave function “no longer represents a pure outgoing wave . . . but . . . contains an $O(\varepsilon)$ component of an incoming wave as well” [1].

We shall be able to show that while the deformations caused by the use of the locally non-Hermitian interaction remain long-ranged in their character, they need not necessarily lead to the emergence of spurious components in the outcoming wave. Such an observation is not in contradiction with the fact that “one should change the Hilbert space by adopting the appropriate metric [which] must differ from the standard one not only in the vicinity of the non-Hermitian potentials, but also at distances remote from it” [1]. Nevertheless, we shall argue that at least some of the spuriousities emerge only due to an inappropriate choice of a specific metric, the definition of which is known to contain infinitely many free parameters [4, 11, 13]. In this sense we shall make use of a simpler model and recommend here the construction and use of another, quasi-local metric operator $\Theta = \Theta^{(QL)} \neq \eta$.

3 Discrete Schrödinger equations

Some of the standard scattering-theory considerations can be simplified when one replaces the ordinary differential equation (1) by the difference equation

$$-\frac{\psi(x_{k-1}) - 2\psi(x_k) + \psi(x_{k+1})}{h^2} + V(x_k)\psi(x_k) = E\psi(x_k).$$

For example, in some pragmatic numerical calculations one chooses a sufficiently small step-size $h > 0$ and introduces discrete coordinates,

$$x_k = k h, \quad k = 0, \pm 1, \ldots .$$

This makes the usual real line replaced or approximated by an infinitely long discrete lattice. The most elementary application of such a discretization occurs when one wants to construct bound states. For certain real as well as complex potentials a sample of the construction may be found in our papers [14]. Some of them illustrate also the fundamental-theory approach to the non-Hermitian quantum bound states where the Hamiltonian $H$ is treated as quasi-Hermitian, i.e., Hermitian only in the Hamiltonian-dependent Hilbert space $\mathcal{H}^{(physical)}$.
3.1 Discrete in and out free waves

Let us assume that the potential in eq. (10) vanishes beyond certain not too large distance from the origin, \( V(x_{\pm j}) = 0, \ j = M, M + 1, \ldots \). In the free-motion domain, we abbreviate \( \psi_j = \psi(x_j) \) and \( 2 \cos \varphi = 2 - h^2 E \) and replace eq. (10) by recurrences

\[
- \psi^{(0)}_{j-1} + 2 \cos \varphi \psi^{(0)}_j - \psi^{(0)}_{j+1} = 0
\]  

(12)

or by the matrix equations \( H_0 \vec{\psi}^{(0)} = h^2 k^2 \vec{\psi}^{(0)} \) or \( M_0(\varphi) \vec{\psi}^{(0)} = 0 \), viz.,

\[
\begin{pmatrix}
\ddots & \ddots & \ddots & \ddots & \ddots & \\
\ddots & 2 \cos \varphi & -1 & 0 & \ldots & \\
\ddots & -1 & 2 \cos \varphi & -1 & \ddots & \\
\ddots & 0 & -1 & 2 \cos \varphi & \ddots & \\
\vdots & \ddots & \ddots & \ddots & \ddots & \\
\end{pmatrix}
\begin{pmatrix}
\psi^{(0)}_{j-1} \\
\psi^{(0)}_j \\
\psi^{(0)}_{j+1} \\
\vdots
\end{pmatrix}
= 0
\]  

(13)

which may be assigned a doublet of independent solutions,

\[
\psi^\pm_k = \text{const} \cdot \varrho_k^\pm, \quad \varrho^\pm = \exp(\pm i \varphi).
\]

Precisely in the spirit of ref. [5] we can speak about a \( \mathcal{PT} \)-symmetric free Hamiltonian,

\[
H_0 = \begin{bmatrix}
\ddots & \ddots & \ddots & \ddots & \\
\ddots & 2 & -1 & \ldots & \\
-1 & 2 & -1 & \ddots & \\
-1 & 2 & \ddots & \ddots & \\
\ddots & \ddots & \ddots & \ddots & \\
\end{bmatrix}, \quad \mathcal{P} = \begin{bmatrix}
1 & \ddots & \ddots & \ddots & \ddots & \\
\ddots & 1 & \ddots & \ddots & \ddots & \\
\ddots & \ddots & 1 & \ddots & \ddots & \\
\ddots & \ddots & \ddots & 1 & \ddots & \\
\ddots & \ddots & \ddots & \ddots & \ddots & \\
\end{bmatrix}.
\]

It is easy to verify that its spectrum is real, provided only that the new energy variable \( \varphi \) is real [8]. This imposes an inessential constraint \(-2 \leq 2 - h^2 E \leq 2\) upon the energy range, i.e., we must have \( E \in (0, 4/h^2) \). At any finite choice of the lattice step \( h > 0 \) this is reminiscent of the similar feature of the spectra in relativistic quantum systems. This connection has been given a more quantitative interpretation in ref. [15].
Let us finally add an interaction with nonzero elements forming merely a finite-dimensional submatrix in the Hamiltonian. The scattering of an incoming wave may be then characterized, say, by the boundary conditions

$$\psi(x_m) = \begin{cases} e^{im\varphi} + R e^{-im\varphi}, & m \leq -M, \\ T e^{im\varphi}, & m \geq M - 1 \end{cases}$$

i.e., by eq. (2) in its discrete version.

### 3.2 Discrete short-range model of scattering

In a way inspired by our recent studies of finite-dimensional non-Hermitian Hamiltonian matrices $H$ with real spectra \cite{8,16} let us pick up one of these models and contemplate its infinite-dimensional generalization which would admit scattering solutions. Its explicit matrix representation will be tridiagonal, one-parametric and doubly infinite,

$$H_1 = \begin{bmatrix} \ddots & \ddots & \ddots & \ddots \\ \ddots & 2 & -1 & \ddots \\ \ddots & -1 & 2 & -1 \\ -1 & 2 & \ddots & \ddots \\ \ddots & \ddots & \ddots & \ddots \end{bmatrix}. \quad (15)$$

Inside the interval of $a \in (-1, 1)$ all the $2K-$dimensional truncations of $H_1$ have the $2K-$plets of eigenvalues which are all real and lie inside the closed interval $(1, 3)$. In the non-Hermitian regime with the growing $|a|$ these energies pairwise degenerate at the “exceptional points” $a = \pm 1$ and get complex at $|a| > 1$. At $K = 2$ and $K = 3$ the smoothness of the $a-$dependence of these truncation-dependent standing wave energies has been illustrated in \cite{8}. At $K = 1$ their explicit form reads $h^2k^2_{\pm} = 3 \pm \sqrt{1-a^2}$ and offers a schematic guidance and a nice quantitative illustration of what happens in general.
In a search for the transmission and reflection amplitudes our infinite-dimensional matrix problem for scattering \( H_1 \psi^{(1)} = \hbar^2 k^2 \psi^{(1)} \) can be split in its two free-motion parts (13) for the respective “in” and “out” solutions (14) valid up to \( M = 1 \). They have to be matched near the origin,

\[
\begin{bmatrix}
-1 & e^{i\varphi} + e^{-i\varphi} & 0 & -1 - a \\
0 & -1 + a & e^{i\varphi} + e^{-i\varphi} & -1
\end{bmatrix}
\begin{bmatrix}
R e^{2i\varphi} \\
R e^{i\varphi} \\
T \\
T e^{i\varphi}
\end{bmatrix}
= \begin{bmatrix}
1 & -e^{i\varphi} - e^{-i\varphi} \\
1 & 1 - a \\
0 & 1 - a \\
0 & e^{-i\varphi}
\end{bmatrix}
\begin{bmatrix}
e^{-2i\varphi} \\
e^{2i\varphi}
\end{bmatrix}.
\]

These two linear equations for \( R \) and \( T \) can be simplified,

\[
\begin{bmatrix}
1 \\
-1 \cdot \frac{1}{(1 - a)e^{i\varphi}}
\end{bmatrix} R + \begin{bmatrix}
-(1 + a) \\
-(1 + a) e^{-i\varphi}
\end{bmatrix} T = \begin{bmatrix}
-1 \\
(1 - a) e^{-i\varphi}
\end{bmatrix}.
\]

It is easy to write down their explicit solution,

\[
R = -\frac{a^2}{\Delta}, \quad T = \frac{(1 - a)(1 - e^{2i\varphi})}{\Delta}, \quad \Delta = 1 - (1 - a^2) e^{2i\varphi}.
\]

This gives an exact analogue

\[
|R|^2 + |T|^2 = \frac{1 - a [1 + U(a, \varphi)]^{-1}}{1 + a [1 + U(a, \varphi)]^{-1}}, \quad U(a, \varphi) = \frac{a^4}{2 (1 - a) (1 - \cos 2\varphi)}
\]

of equation Nr. (11) of ref. [1]. In both cases, the sum of probabilities is greater than 1 or less than 1 depending on the sign of the deviation of the coupling constant form its Hermitian zero limit. The same conclusion can be read in ref. [1] so that in the weak-coupling regime our present difference-operator parameter \( a \) plays the same dynamical role as its differential-operator predecessor \( \varepsilon \) in eq. (5). Moreover, due to the nonperturbative character of our result one can rewrite eq. (16) in the equivalent form [17]

\[
|R|^2 + |T|^2 = \frac{a^4 + 4(1 - a)^2 \sin^2 \varphi}{a^4 + 4(1 - a^2) \sin^2 \varphi}
\]

which is more compact and clarifies the nature of the singularity reached in the limit \( a \to 0 \).

We shall also see below (cf. section 4.2) that after the necessary adaptation of the Hilbert space of states and after the \textit{ad hoc} modification of the inner product the net
result of the changes will be the elementary modification of the coefficient of \(\sin^2 \varphi\) in the numerator to \(4(1 - a^2)\), thus restoring the usual and physically consistent unitarity of the scattering.

### 3.3 More-parametric models

With another Hamiltonian

\[
H_2 = \begin{bmatrix}
\ddots & & & & & \\
& 2 & -1 & & & \\
& -1 & 2 & -1 - b & & \\
& & -1 + b & 2 & -1 - a & \\
& & -1 + a & 2 & -1 - b & \\
\ddots & & & & & \\
\end{bmatrix}
\]

one can expect that many results obtained previously for its \(b = 0\) special case \(H_1\) can find a natural generalization. The same expectations concern also the next-step candidate with three free parameters,

\[
H_3 = \begin{bmatrix}
\ddots & & & & & \\
& -1 & 2 & -1 - c & & \\
& -1 + c & 2 & -1 - b & & \\
& & -1 + b & 2 & -1 - a & \\
& & -1 + a & 2 & -1 - b & \\
& & & -1 + b & 2 & -1 - c & \\
& & & & -1 + c & 2 & -1 & \\
\ddots & & & & & & \\
\end{bmatrix}
\]

etc. In all of them the asymptotic “in” and “out” solutions of eq. (14) remain uninfluenced by the interaction. Equally well, the matching of these in and out solutions remains feasible at any number \(k\) of parameters.
In our first nontrivial scattering model \( H_2 \vec{\psi}^{(2)} = \hbar^2 k^2 \vec{\psi}^{(2)} \) the matching may be mediated by the choice of \( M = 2 \). This means that the following four matching conditions must be considered,

\[
\begin{bmatrix}
-1 & 2 \cos \varphi & -1 - b & 0 & 0 & 0 \\
0 & -1 + b & 2 \cos \varphi & -1 - a & 0 & 0 \\
0 & 0 & -1 + a & 2 \cos \varphi & -1 - b & 0 \\
0 & 0 & 0 & -1 + b & 2 \cos \varphi & -1 \\
\end{bmatrix}
\begin{bmatrix}
e^{-3i\varphi} + R e^{3i\varphi} \\
e^{-2i\varphi} + R e^{2i\varphi} \\
e^{-i\varphi} + R e^{i\varphi} - \chi_{-1} \\
T + \chi_0 \\
T e^{i\varphi} \\
T e^{2i\varphi} \\
\end{bmatrix}
= 0.
\]

The first line defines the correction \( \chi_{-1} \) and the last line defines the correction \( \chi_0 \),

\[
(1 + b) \chi_{-1} = b (e^{-i\varphi} + R e^{i\varphi}), \quad (1 - b) \chi_0 = b T.
\]

This reduces the number of our equations to two again,

\[
\begin{bmatrix}
-1 + b & 2 \cos \varphi & -1 - a & 0 \\
0 & -1 + a & 2 \cos \varphi & -1 - b \\
\end{bmatrix}
\begin{bmatrix}
e^{-2i\varphi} + R e^{2i\varphi} \\
(e^{-i\varphi} + R e^{i\varphi}) / (1 + b) \\
T / (1 - b) \\
T e^{i\varphi} \\
\end{bmatrix}
= 0.
\]

After their simplification we may easily eliminate

\[
\frac{(1 + b) T}{(1 - a)(1 - b)} = \frac{1 + R e^{2i\varphi}}{1 + b^2 e^{2i\varphi}}.
\]

We end up quickly with the explicit definition of \( R \) for our second model \( H_2 \),

\[
R = -\frac{a^2 + 2 b^2 \cos 2 \varphi + b^4}{\Delta}, \quad \Delta = 1 - (1 - a^2) e^{2i\varphi} + 2 b^2 e^{2i\varphi} + b^4 e^{4i\varphi}.
\]

We observe a close parallelism with the preceding model. From the easy first-order estimates

\[
R = \mathcal{O}(a^2) + \mathcal{O}(b^2), \quad \frac{(1 + b) T}{(1 - a)(1 - b)} = 1 + \mathcal{O}(a^2) + \mathcal{O}(b^2)
\]

we may immediately deduce that

\[
|R|^2 + |T|^2 = 1 - 2 a - 4 b + \mathcal{O}(a^2) + \mathcal{O}(b^2).
\]
4 Unitarily non-equivalent Hilbert spaces

In a climax of our paper we shall make use of the fact that our models are exactly solvable, at least in terms of the methods based on the computer-assisted symbolic manipulations and extrapolations. This will enable us to construct many eligible candidates $\Theta$ for the metric in the physical Hilbert space. In contrast, even the construction of their subclass denoted by the symbol $\rho$ and possessing an explicit perturbation form

$$\rho = I + \frac{1}{2} \varepsilon \eta^{(1)} + \mathcal{O}(\varepsilon^2).$$

was an achievement for differential operators in refs. [1] and [9]. In such a context, a core of our present message is that due to the simplified, difference-operator representation of observables we shall be able to select a better metric $\Theta^{(QL)} \neq \eta$. With its use, some of the most counterintuitive manifestations of the nonlocality paradox will simply disappear.

4.1 Ambiguity problem

In the effective interaction scenario, formulae (6) or (16) and (18) would certainly indicate the presence of an absorption and/or creation at $\varepsilon \neq 0$ or $a \neq 0$ and $b \neq 0$.

In the fundamental theory one assumes a change of the Hilbert space such that the original (i.e., standard) definition of the inner product

$$\langle \psi | \psi' \rangle = \int_{\mathbb{R}} \psi^*(x) \psi(x) \, dx$$

is replaced by its more general weighted version in the new space,

$$\langle \psi | \psi' \rangle_{\Theta} = \int_{\mathbb{R}^2} \psi^*(x) \Theta(x, x') \psi'(x') \, dx \, dx'. \quad (21)$$

The purpose of such a change is in making the Hamiltonian selfadjoint.

It is well known that the choice of the inner product (21) is ambiguous [4]. One of the standard constructive solutions of the ambiguity problem giving $\Theta = \eta$ has been proposed by Mostafazadeh [9]. In the mathematically most easily tractable dynamical regime of a very small deviation $|\varepsilon| \ll 1$ from Hermiticity this author
arrived at the explicit perturbation approximation (8) + (9) where the maxima of function \( \eta(x, y) \) lie on the two perpendicular lines defined by the trivial equations \( x \pm y = 0 \) in the \( x-y \) plane. Subsequently, the latter recipe has been used in ref. [1] where operator \( \Omega^{(Jones)} \equiv \rho \) was defined as a self-adjoint square root (19) of metric \( \eta \) emphasizing that in terms of physics, “the relevant wave function is not \( \psi(x) \equiv \langle x|\psi \rangle \), but \( \Psi(x) \equiv \langle x|\Psi \rangle = \langle x|\rho|\psi \rangle \).”

In this context, the mathematical essence of our present amendment of scattering theory lies precisely in an innovation of the choice of \( \Omega \) and \( \Theta \) since among all the available mappings \( \Omega \) the selected \( \rho \) remains also very strongly non-local, indeed.

4.2 The existence of diagonal matrices \( \Theta = \Theta^{(QL)} \)

In the technically most complicated part of our present considerations we decided to choose a Hamiltonian and to treat its quasi-Hermiticity condition (7) as a linear set of equations for all the matrix elements of the metric.

In the first attempt we choose \( H_1 \) and verified that there exists the infinite-dimensional matrix solution \( \Theta_1 \) of eq. (7) which is diagonal, i.e., in our present terminology, quasi-local,

\[
\Theta_1^{(QL)} = \begin{bmatrix}
\ddots & 1 - a & & \\
& 1 - a & & \\
& & 1 - a & \\
& & & 1 + a \ddots
\end{bmatrix}.
\]

This result was obtained via tedious symbolic manipulations on the computer. Its simplicity is both very surprising and very useful because one of the integrations in the related inner product (21) drops out. Moreover, its diagonal kernel can trivially
be factorized into the product of two diagonal operators \( \rho = \sqrt{\Theta} \), i.e.,

\[
\rho^{(QL)}_1 = \begin{pmatrix}
\cdots & \sqrt{1-a} & \sqrt{1-a} & \sqrt{1-a} & \cdots \\
\sqrt{1-a} & 1 & 1 & 1 & \cdots \\
1 & 1 & 1 & 1 & \cdots \\
\sqrt{1-a} & \sqrt{1-a} & \sqrt{1-a} & \sqrt{1-a} & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots 
\end{pmatrix}
\]

They remain self-adjoint and positive definite at all the not too large real \( a \).

The diagonality of the latter matrix enables us to insert it in eq. Nr. (17) of ref. [1] and to deduce that the explicit formula for the “correct” operator \( X \) of the observable coordinate coincides with its standard diagonal-matrix form with elements given by eq. (11) above. In the same manner one can also recall eq. (4) and introduce the operator 

\[
h^{(QL)}_1 = \rho^{(QL)}_1 H_1 \left( \rho^{(QL)}_1 \right)^{-1}
\]

which represents the isospectral Hermitian Hamiltonian of our system and which replaces eq. (15) by the real and symmetric tridiagonal matrix

\[
h^{(QL)}_1 = \begin{pmatrix}
\cdots & \cdots & \cdots & \cdots & \cdots \\
\cdots & 2 & 1 & \cdots & \cdots \\
1 & 2 & 1 & \cdots & \cdots \\
1 & 2 & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots 
\end{pmatrix}
\]

We see that this operator differs from the purely kinetic Hamiltonian just in a small vicinity of the scattering center. In spite of such a strict locality of the interaction, the metric itself remains deformed far away from the scattering center.

The fact that the manifest non-Hermiticity of our toy model \( H_1 \) did not involve the mixing of incoming and outgoing waves that occurred in the model of ref. [1].
encouraged us to proceed towards the more complicated models using the same brute-force method. After the choice of the next, two-parametric non-Hermitian Hamiltonian $H_2$ the calculations still remained sufficiently easy for us to deduce and verify the existence of the following two-parametric quasi-local solution $\Theta_2^{(QL)}$ of eq. (7) represented by the diagonal matrix

$$
\begin{bmatrix}
\cdots \\
(1 - a) (1 - b)^2 \\
(1 - a) (1 - b)^2 \\
(1 - a) (1 - b^2) \\
(1 - a) (1 - b^2) \\
(1 + a) (1 - b^2) \\
(1 + a) (1 - b^2) \\
(1 + a) (1 + b^2) \\
(1 + a) (1 + b^2) \\
\cdots
\end{bmatrix}
$$

Similarly, we took $k = 3$ in the next continuation of the series of solutions $\Theta_k^{(QL)}$ pertaining to $H_k$. It is easy to verify that the three-parametric quasi-local solution $\Theta_3^{(QL)}$ of eq. (7) is still obtainable as a diagonal matrix with the same elements $(1 - a) (1 - b)^2 (1 - c)^2$ in all the upper left corner and with the similar array of the same elements $(1 + a) (1 + b)^2 (1 + c)^2$ in its lower right corner. The remaining “central” quadruplet of the “anomalous” diagonal elements is formed by the following four-dimensional diagonal central submatrix of our doubly infinite matrix $\Theta_3^{(QL)}$,

$$
\begin{bmatrix}
(1 - a) (1 - b)^2 (1 - c^2) \\
(1 - a) (1 - b^2) (1 - c^2) \\
(1 + a) (1 - b^2) (1 - c^2) \\
(1 + a) (1 + b)^2 (1 - c^2)
\end{bmatrix}
$$

The general pattern of extrapolation is now obvious. It would be easy to write down and, via eq. (7), verify an immediate extrapolation of the $k = 1$, $k = 2$ and $k = 3$ matrices $\Theta_k^{(QL)}$ to the higher subscripts $k$ whenever necessary.

There are all reasons why, in the context of scattering, the specific diagonal metrics $\Theta_k^{(QL)}$ should be preferred in comparison with all their non-diagonal and,
hence, more nonlocal alternatives. With such a new postulate we may now return to paper [1] once more. First of all our results reconfirm the high plausibility of the hypothesis that even the violation of the Hermiticity which is strictly localized in space should be expected to influence, manifestly, even the asymptotics of the wave functions. The explicit analysis of our schematic models indicates that even our minimally nonlocal metric operators remain, strictly speaking, different from the most common Dirac’s delta-function metric $\Theta^{(\text{Dirac})}(x,y) = \delta(x - y)$ at all distances.

This being said, we found it quite fortunate that at the sufficiently large distances, i.e., for $|x| \gg 1$ and/or $|y| \gg 1$, the difference between $\Theta^{(\text{Dirac})}(x,y)$ and $\Theta^{(QL)}_k(x,y)$ degenerated, in all of our models, to the mere introduction of a nontrivial multiplication factor,

$$\Theta^{(QL)}(x,y) = \text{const}(\text{sign } x) \cdot \Theta^{(\text{Dirac})}(x,y), \quad |x| \gg 1, \quad |y| \gg 1. \quad (23)$$

In another formulation, our explicit constructions very strongly support the affirmative answer to the question of the existence of a “spatially localized non-Hermiticity”. A formal key to such an answer is that in a schematic model we constructed certain new and very specific, “quasi-local” metrics $\Theta^{(QL)}$ with the property (23).

The strict validity of this proportionality rule at almost all the coordinates $x$ and $y$ may be admitted to be an artifact resulting from our specific tridiagonal-matrix choice of our “toy” Hamiltonians $H_k$. Still, the validity of such a rule at all the sufficiently large coordinates may be expected to survive transition to a larger family of models and, perhaps, also to some slightly less friendly generalized quasi-linear forms of $\Theta^{(QL)}$, say, with a band-matrix structure. This would still allow us to conjecture that with the metrics $\Theta = \Theta^{(QL)}$ the internal consistency of the models of scattering (and, in particular, of their asymptotic boundary conditions) would not be violated after the extension of the present theory towards many less schematic and reasonably non-Hermitian models of dynamics.

One of the instrumental versions of our conjecture will have the form of the requirement $D' = 0$ in boundary conditions so that eq. (3) $\equiv$ eq. (2). Then, the choice of a unique metric $\Theta^{(QL)}$ characterized by its minimalized nonlocality should
be perceived as strongly recommended in the conceptually consistent fundamental scattering theory using non-Hermitian Hamiltonians.

Marginally, the latter requirement can be supported also by the remark that “it has been known for some time that ... for the potential $ix^3$ and the infinite $\mathcal{PT}$–symmetric square well ... the particle is confined ... so that the range of the non-locality is limited. Scattering potentials highlight this feature [of nonlocality] to its full extent because the wave functions ... do not have compact support.” [1]. This means that the “traditional” choices of $\Theta \neq \Theta^{(QL)}$ can still offer a fully consistent model of the physical reality for bound states. After all, we already noticed that many models with $\Theta \neq \Theta^{(QL)}$ found applications in nuclear physics [4] and in field theory [5]. Other constructions of $\Theta \neq \Theta^{(QL)}$ appeared also in the coupled-channel problems [12] or in the Klein-Gordon-type models [18] etc.

5 Summary

In the differential-equation model of scattering studied in ref. [1] the behavior of the physical “in” and “out” states was strongly non-local so that, for example, the outgoing waves contained a non-negligible “incoming” component. In this context we showed here that such a paradox is not inevitable for non-Hermitian systems with real spectra. A set of counter-examples has been described here in which the local non-Hermiticites carried by the Hamiltonian implied just the necessity of the replacement of the usual scalar product (20) by the local, re-scaling change of the measure,

$$\langle \psi | \psi' \rangle = \int_{\mathbb{R}^2} \psi^*(x) \Theta(x) \psi'(x) \, dx.$$ (24)

This enabled us to address several conceptual difficulties as encountered in ref. [1] where the description of scattering caused by several short-range non-Hermitian sample potentials $V(x)$ has been presented. In this context we discovered and described a family of non-Hermitian short-range Hamiltonians $H_1, H_2, \ldots$ for which the description of the scattering looks almost as easy and natural as in the standard Hermitian regime.
Our selection of short-range interaction models proved technically much simpler than expected. We revealed several amazingly close parallels with their continuous delta-function analogues. We were able to bring new arguments, first of all, thanks to certain “unreasonable efficiency” of our non-perturbative method. In this framework, our main mathematical result is that the hermitizing metrics $\Theta = \Theta_k$ which we attached to $H_1$, $H_2$ and $H_3$ and, by an easy extrapolation, to any $H_k$ are all represented by the (infinite-dimensional) diagonal matrices. We believe that this is not just a friendly feature of our specific models but rather a generic property of the metrics since one has a lot of freedom of their modification in general.

In the latter spirit, our present main recommendation is that for all the realistic non-Hermitian models of scattering one should still try to insist on the requirement that the physical metric $\Theta$ is not too non-local. In our present text we succeeded in supporting the latter recommendation by a series of the explicit illustrations of its feasibility. One of reasons was that we choose the discretization of the real line of coordinates as our principal methodical tool.

The first hints offering a background for such a decision were already found and formulated in [8]. The present results can briefly be characterized as a successful transition from the bound-state models (or, formally, from the finite $N$−point lattices of ref. [14]) to the scattering scenario (or, formally, to the limit $N \to \infty$), complemented by the replacement of the simplest possible one-parametric model of ref. [8] by the whole set of dynamically nontrivial localized Hamiltonians $H_k$ containing, in principle, an arbitrary finite number $k$ of coupling constants.

A formal benefit of our choice of the models appeared to lie in their two-faced solvability. Its first face was rather technical and concerned an easiness of construction of the reflection and transition coefficients. Certain massive cancellations in the linear algebraic matching conditions made the final formulae unbelievably compact. The second friendly face of the solvability emerged during our systematic construction of the metrics $\Theta$. An easiness of the guesswork encountered during extrapolations $k \to k + 1$ is worth mentioning since it proved helpful and saved computer time.

A priori we couldn’t have hoped in the amazing diagonality of our solutions
of eq. (7) or in their asymptotically constant form or in a “user-friendliness” of the transition from the trivial model $H_k$ with $k = 1$ to virtually all of its $k > 1$ descendants. We firmly believe that at least some of these properties will also be encountered in some other, similar but less schematic models of the dynamics.

Needless to add that many emerging questions remain open. Some of them (like, typically, the numerical efficiency of the discretizations and an analysis of the practical rate of their convergence) have been skipped intentionally. The omission of some other points was only made with regret, mainly because of their lack of any immediate relevance for physics. For example, a marginal but interesting benefit of the discretization with a fixed gap $h > 0$ could have been seen in the emergence of parallelism between the discrete-lattice formulae and their continuous-limit counterparts. Besides such a direct possible correspondence between $H_k$s and point interactions, another correspondence (viz., to the truncated, finite lattices) has also been omitted as too mathematical, in spite of its potential relevance for the verification of the reality of the spectra.

We are sure that even within the domain of physics we did not list all the open questions. *Pars pro toto*, let us sample, in the conclusion, the possible relevance of the present models with the extremely simple metrics in the context of the path-integral formulation of Quantum Theory where an extremely interesting discussion just appears in print [19], concerning the questions of the role of the explicit form of the metric $\Theta$ in the partition functions $Z[J]$ and in certain related formulae in thermodynamics and/or quantum field theory.

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