Pseudo-Hermitian approach to energy-dependent Klein-Gordon models

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Abstract
The relativistic Klein-Gordon system is studied as an illustration of Quantum Mechanics using non-Hermitian operators as observables. A version of the model is considered containing a generic coordinate- and energy-dependent phenomenological mass-term $m^2(E, x)$. We show how similar systems may be assigned a pair of the linear, energy-independent left- and right-acting Hamiltonians with quasi-Hermiticity property and, hence, with the standard probabilistic interpretation.

KEYWORDS: Quantum Mechanics; energy-dependent forces; pseudo- and quasi-Hermitian formalism; relativistic kinematics; linear representation of observables

1 Introduction
In units $\hbar = c = 1$ Quantum Mechanics describes the motion of a free spinless particle by the partial (parabolic) differential Schrödinger equation

$$i \partial_t \psi = -\frac{1}{2m} \Delta \psi$$

or, in the relativistic kinematical regime, by the hyperbolic Klein-Gordon equation

$$(i \partial_t)^2 \psi = (-\Delta + m^2) \psi.$$  

Various phenomenological requirements may be met via an introduction of a suitable time-independent interaction which still admits the usual formal Fourier-transformation separation of the time-dependence.
We intend to contemplate a generic situation where the form of the interaction is allowed to vary with the energy. A schematic clarification of a few basic features of the models of this type may be offered by the Schrödinger equation (1) where we may put \( \psi = \psi(t) = e^{-iEt}\Psi(r) \) and postulate the most elementary harmonic-oscillator form of the interaction. In one dimension this leads to the ordinary differential equation

\[
-\frac{1}{2m(E)} \frac{d^2}{dr^2} \Psi(r) + r^2 \Psi(r) = E \Psi(r)
\]  

(3)

where a few possible effects of the variability of the mass with the energy may be illustrated by the most elementary ansatz \( 2m(E) = A^2 (E - E_0)^2 \). A mere rescaling of eq. (3) leads to the solvable bound-state problem with the spectrum determined by the closed formulae

\[
E = \begin{cases} 
E_n^{(+)} = E_0 + \sqrt{E_0^2 + (8n + 4)/A}, & n = 0, 1, \ldots, \\
E_{\pm n}^{(-)} = E_0 \pm \sqrt{E_0^2 - (8n + 4)/A}, & n = 0, 1, \ldots, n_{\text{max}}. 
\end{cases}
\]  

(4)

The unusual second family is finite and remains non-empty only for \( AE_0^2 \geq 4 \). New levels emerge at each new \( n_{\text{max}} = \text{entier}[(AE_0^2 - 4)/8] \).

### 1.1 Relativistic kinematics as a challenge in physics

Our intuition may fail in similar situations, indeed. In a way complementing the recent study of nonrelativistic energy-dependent descendants of eq. (1) [1], we intend to pay attention to the relativistic models where the standard Klein-Gordon Hamiltonians (= the operators of energy) do not coincide with the generators of time evolution [2].

This is a challenging difficulty. In addition we see an even stronger reason for interest in Klein-Gordon system in its close connection to an extended Quantum Mechanics using non-Hermitian operators [3]. Thus, we are going to pay attention to the relativistic Klein-Gordon equations

\[
(i \partial_t)^2 \Psi^{(KG)}(x, t) = \hat{H}^{(KG)} \Psi^{(KG)}(x, t)
\]  

(5)

with interactions mediated by a coordinate- and energy-dependence of the phenomenological mass-term in \( \hat{H}^{(KG)} = -\Delta + m^2(E, x) \).
1.2 Non-Hermiticity of Hamiltonians as a challenge in mathematics

It is well known [4] that the usual Klein-Gordon Hamiltonians $\hat{H}^{(KG)}$ are pseudo-Hermitian or, in a more compact wording, $PT-$symmetric [5]. The latter type of symmetry emerged in Quantum Mechanics as related to the imaginary cubic (cf. [6]) or negative quartic (cf. [7]) anharmonicities, with important implications expected also within the relativistic Quantum Field Theory [8]. Nevertheless, its key importance has only been revealed and emphasized by Bender and Boettcher [5] who conjectured that the enigmatic reality of spectra of certain nonrelativistic Hermiticity-violating oscillators might be attributed to an unusual commutativity of their Hamiltonians with the product $PT$ of parity $P$ and time reversal $T$.

Later on, it became clear that all the similar models (with both the purely real or mixed, complex-conjugate spectra) seem to obey an unusual, pseudo-unitary time-evolution law [9] reflecting the pseudo-Hermiticity of the Hamiltonian. One had to return to the older work by Dirac et al [10] to imagine that the self-adjoint and invertible operator $P$ replaces the usual identity operator in the role of an indeterminate pseudo-metric in the Hilbert space. In some exactly solvable examples the puzzling indeterminacy of the corresponding pseudo-norm has been attributed to the mere sign-type variable called quasi-parity [11] or, later but much better, charge $C$ [12].

Ali Mostafazadeh [13] realized that formally, there are no real reasons against the replacement of the indeterminate pseudo-metric $P$ (or $\eta$ in his - or rather Dirac’s - preferred notation) by an “equivalent” (though still in general non-unique) positive-definite “physical” metric $\eta_+$ which, in essence, coincides with the operator $CP$ of ref. [12] and admits the current probabilistic interpretation of the theory.

It is amusing to notice that at the moment of its introduction, the operator $\eta_+ > 0$ itself has already been used and studied for more than ten years, within the framework of nuclear physics. In the review paper by Scholtz et al [14], the name “quasi-Hermitian” has been coined for all the “physically consistent” (i.e., in the present language, $CPT-$symmetric [12]) observables, i.e., for all the operators $H$ such that $H^\dagger = \eta_+ H \eta_-^{-1}$ in the notation of ref. [13]. As long as $\eta_+$ varies, in general, with the Hamiltonian, its construction, trivial as it may seem in some exactly solvable examples [15], represents a really formidable task in the majority of the complicated models of Quantum
2 Klein-Gordon models

2.1 Pseudo-Hermiticity

We intend to show how the nonlinearity caused by the energy dependence may be suppressed by the separation of the left- and right-action of the Hamiltonian. In (5) we abbreviate $\Psi^{(KG)}(x,t) = \varphi_2^{(SR)}(x,t)$ and $i \partial_t \Psi^{(KG)}(x,t) = \varphi_1^{(SR)}(x,t)$ and get the following Schrödinger-type re-arrangement of our equation,

$$i \partial_t \begin{pmatrix} \varphi_1^{(SR)}(x,t) \\ \varphi_2^{(SR)}(x,t) \end{pmatrix} = \hat{h}^{(SR)} \cdot \begin{pmatrix} \varphi_1^{(SR)}(x,t) \\ \varphi_2^{(SR)}(x,t) \end{pmatrix}, \quad \hat{h}^{(SR)} = \begin{pmatrix} 0 & \hat{H}^{(KG)} \\ 1 & 0 \end{pmatrix}.$$

As long as the concept of pseudo-Hermiticity of an operator $A$ requires just the fulfillment of the operator relation $A^\dagger = \eta A \eta^{-1}$, the “pseudo-metric” operator $\eta = \eta^\dagger$ is, in general, indeterminate and $A$-dependent. Still, we may immediately assume the pseudo-Hermiticity of the energy operator,

$$\left(\hat{H}^{(KG)}\right)^\dagger = \eta^{(KG)} \hat{H}^{(KG)} \left(\eta^{(KG)}\right)^{-1},$$

and note that it implies that

$$\left(\hat{h}^{(SR)}\right)^\dagger = \eta^{(SR)} \hat{h}^{(SR)} \left(\eta^{(SR)}\right)^{-1}, \quad \eta^{(SR)} = \begin{pmatrix} 0 & \eta^{(KG)} \\ \eta^{(KG)} & 0 \end{pmatrix},$$

i.e., it already guarantees the pseudo-Hermiticity of the generator $\hat{h}^{(SR)}$ of the time evolution.

2.2 Quasi-Hermiticity

In the spirit of paragraph 1.2 we must perform the second step and replace both the generalized parities $\eta^{(SR)} = P^{(SR)}$ and $\eta^{(KG)} = P^{(KG)}$ by the respective positive, “physical” metric operators $\eta_+^{(SR)} = C^{(SR)} P^{(SR)}$ and $\eta_+^{(KG)} = C^{(KG)} P^{(KG)}$. This means that the corresponding scalar products as well as the norms will behave in such a manner that the axioms of Quantum Mechanics remain satisfied. In the other words, our operators become
“Hermitian” whenever we decide to understand the “Hermiticity” in the new metric $\eta^{(SR)}_+ \equiv C^{(SR)}p^{(SR)}$. In this sense, also the time-evolution of the Klein-Gordon system remains “unitary” in the new language.

3 Separation of the left and right action of the Hamiltonians

3.1 Bi-orthogonal bases and energy as a parameter

In any energy-dependent interaction term, we may tentatively replace the variable energy $E$ by a fixed parameter $z$ and compute the whole spectrum $E(z)$ of each $H(z)$ at any value of $z$. This gives us a family of auxiliary spectral decompositions

$$H(z) = \sum_n |\Psi^{(n)}(z)\rangle E^{(n)}(z) \langle \Psi^{(n)}(z)|.$$  \hspace{1cm} (6)

Thus, our pseudo-Hermitian input Hamiltonians $H(z)$ are, in the light of the current textbooks [18], easily tractable as matrices in a suitable bi-orthogonal (or rather bi-orthonormal) basis. This means that

$$\langle \Psi^{(m)} | \Psi^{(n)} \rangle = \delta^n_m, \hspace{1cm} m, n = 1, 2, \ldots$$

while the completeness relations may also be assumed in the form of the infinite series,

$$\hat{I} = \sum_n |\Psi^{(n)}\rangle \langle \Psi^{(n)}|.$$  \hspace{1cm} (7)

In the light of the pseudo-Hermiticity rules we may write

$$H^\dagger \eta = \eta H = \sum_n |\Psi^{(n)}\rangle E^{(n)} \langle \Psi^{(n)}|, \hspace{1cm} \eta = \sum_n |\Psi^{(n)}\rangle \langle \Psi^{(n)}| = \eta^\dagger,$$  \hspace{1cm} (8)

$$H \eta^{-1} = \eta^{-1} H^\dagger = \sum_n |\Psi^{(n)}\rangle E^{(n)} \langle \Psi^{(n)}|, \hspace{1cm} \eta^{-1} = \sum_n |\Psi^{(n)}\rangle \langle \Psi^{(n)}|.$$  \hspace{1cm} (9)

Whenever the metric is positive, $\eta > 0$ we may call our Hamiltonians quasi-Hermitian. In an error-checking convention of ref. [1] we may also temporarily consider only the formulae where all the kets and bras are upper- and lower-indexed, respectively.
3.2 Innovated bi-orthogonal bases

Once we return to the implicit constraint

\[ z_{\text{phys}} = E^{(n)}(z_{\text{phys}}) \]  \hspace{1cm} (10)

and to its explicit solutions

\[ z_{\text{phys}} = E^{(n,1)}, E^{(n,2)}, \ldots, E^{(n,m(n))} \]

we have to move to a new basis. Thus, we denote

\[ |\Psi(n)_{\text{phys}}\rangle = |\phi_\alpha\rangle \]

and abbreviate

\[ E^{(n,j)} = E_\alpha \] using multi-indices \( \alpha = (n,j) \). All the overlaps are assumed calculable,

\[ \langle\varphi_\alpha|\varphi_\beta\rangle = R_\beta^\alpha. \]

This suffices for a formal representation of the unit projector,

\[ \hat{I} = \sum_{\alpha,\beta \in A} |\varphi_\alpha\rangle \langle\varphi_\alpha| = \sum_{\beta \in A} |\varphi_\beta\rangle \langle\varphi_\beta| = \sum_{\alpha \in A} |\varphi_\alpha\rangle \langle\varphi_\alpha| \] \hspace{1cm} (11)

with abbreviations

\[ \sum_{\alpha \in A} |\varphi_\alpha\rangle \langle\varphi_\alpha| = |\varphi^\alpha\rangle \], \hspace{1cm} \sum_{\beta \in A} \langle\varphi_\beta|\varphi_\beta\rangle = \langle\varphi_\beta|\varphi_\beta\rangle = \delta_\beta^\alpha. \]

and with the innovated completion relations

\[ \hat{I} = \sum_{\alpha \in A} |\varphi_\alpha\rangle \langle\varphi_\alpha| = \sum_{\alpha \in A} |\varphi_\alpha\rangle \langle\varphi_\alpha|. \]

4 The elimination of the energy dependence

Two alternative tentative spectral expansions of our quasi-Hermitian \( H(E) \) read

\[ K = \sum_{\alpha \in A} |\varphi_\alpha\rangle E_\alpha \langle\varphi_\alpha|, \hspace{1cm} L = \sum_{\beta \in A} |\varphi_\beta\rangle E_\beta \langle\varphi_\beta|. \]

These operators share the action of \( H(E) \) to the right and to the left, respectively,

\[ K |\varphi_\beta\rangle = E_\beta |\varphi_\beta\rangle, \hspace{1cm} \langle\varphi_\alpha| L = E_\alpha \langle\varphi_\alpha|. \]
They are both energy-independent – this is their main merit. Their quasi-Hermiticity rules acquire the form

$$K^\dagger \mu = \mu K = \sum_{\alpha \in A} |\varphi_\alpha\rangle \langle \varphi_\alpha| E_\alpha, \quad \nu L = L^\dagger \nu = \sum_{\alpha \in A} |\varphi_\alpha\rangle \langle \varphi_\alpha| E_\alpha,$$

where one has to abandon the above-mentioned “error-correcting” convention,

$$\mu = \sum_{\alpha \in A} |\varphi_\alpha\rangle \langle \varphi_\alpha| = \mu^\dagger, \quad \nu = \sum_{\alpha \in A} |\varphi_\alpha\rangle \langle \varphi_\alpha| = \nu^\dagger.$$

These Klein-Gordon related formulae complement and extend their nonrelativistic predecessors of ref. [1]. We may summarize our considerations by saying that the transition to the relativistic kinematics requires a weaker (viz., pseudo- or quasi-) Hermiticity of the initial (= Feshbach-Villars-type) Hamiltonians $H_{(SR)}(E)$. The bra and ket vectors in the spectral expansions cease to be the mere Hermitian conjugates of each other because they are formed by the two sets of eigenstates of $H$ and $H^\dagger$ [1]. Still, the work in these bi-orthogonal bases remains extremely natural, both before and after the introduction of an energy dependence in our interactions. In this sense, the formal differences between the nonrelativistic and relativistic models appear to be minimal.

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