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Quantum Mechanics of Klein-Gordon equation

MASTER THESIS

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V Praze dne ....

....
Bc. Iveta Semorádová

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Název práce:
Kvantová mechanika Kleinovy-Gordonovy rovnice

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Abstrakt: Zkoumáme Kleinovu-Gordonovu rovnici v novém rámci kvazihermitovské kvantové mechaniky. Je navrženo řešení běžných problémů s pravděpodobnostní interpretací a indefinitním skalárním součinem Kleinovy-Gordonovy rovnice. Počítáme metrický operátor jak pro diferenciální, tak pro diskrétní případy. Kvazihermitovská kvantová teorie je podrobně shrnuta včetně problému časového vývoje kvantového systému s časově závislou metrikou. Využití 1/L poruchové metody pro Schrödingerovu formu Kleinovy-Gordonovy rovnice se ukázalo jako efektivní.

Klíčová slova: relativistická kvantová mechanika, Klein-Gordonova rovnice, pravděpodobnostní interpretace, 1/L poruchová metoda, metrický operátor, kryptohermitovký operátor, kvazihermitovský operátor

Title:
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Abstract: We explore Klein-Gordon equation in the new framework of quasi-Hermitian quantum mechanics. Solutions to common problems with probability interpretation and indefinite inner product of Klein-Gordon equation are proposed. We compute metric operators for differential as well as discrete case. Thorough summary of quasi-Hermitian quantum theory is presented including the problem of time evolution of the quantum system with time-dependent metric. The use of 1/L perturbation method for the Shrödinger form of Klein-Gordon equation is shown efficient.

Key words: relativistic quantum mechanics, Klein-Gordon equation, probability interpretation, 1/L perturbation method, metric operator, crypto-Hermitian operator, quasi-Hermitian operator

Content

List of symbols

$\mathcal{H}$	...	separable Hilbert space
$\mathbb{C}^N$	...	Hilbert space of N-tuples of complex numbers
ℓ_2	...	Hilbert space of all sequences $\{\xi_j\}_{j=1}^{\infty}$, such as $\sum_{j=1}^{\infty} \|\xi_j\|^2 < \infty$
$L^2(\mathbb{R}^3)$	...	Hilbert space of square integrable functions on $\mathbb{R}^3$
$\vec{a}$	...	vector
a	...	four-vector
$a.b$	...	scalar product of four-vectors
∇	...	nabla operator
Δ	...	Laplace operator
$\Box$	...	d'Alembert operator
∂_x	...	partial derivative with respect to x
δ_{mn}	...	Kronecker delta
$\delta(\vec{k})$	...	Dirac delta function
Θ	...	metric operator
Ω	...	similarity operator, Dyson's map
H	...	linear operator
K	...	positive Hermitian operator
iff	...	if and only if
$D(H)$	...	domain of linear operator H

Introduction

Ninety years ago the problem of proper probability interpretation of Klein-Gordon equation arised. Its indefinite probability density function allows existence of both positive and negative probabilities, which obstructs its proper physical interpretation. In 1934 Pauli and Weisskopf [46] solved the problem by reinterpreting Klein-Gordon equation in the context of quantum field theory. Field equation was satisfied by an operator $\phi(x)$, which was not a wave function but a quantum field, whose excitations may be an arbitrary number of particles. Negative energy states were reinterpreted as antiparticles and indefinite probability density ρ started to play role of the charge density. Klein-Gordon equation is considered a suitable equation for spinless particles, such as pions, described by spinless scalar field [45].

The idea of treating Klein-Gordon equation in quantum mechanical context only without further field consideration was forgotten. This subject was brought back in 2003 by Ali Mostafazadeh [38] who used the knowledge of pseudo-Hermitian quantum mechanics to introduce proper probability interpretation of Klein-Gordon equation. Metric operator defining positive definite inner product on the solution space of free Klein-Gordon operator was successfully counted. Several publications concerning this subject appeared [39, 43, 44, 40] or [56, 57, 67]. But the topic was left with lots of room left for deeper exploration. There are wide possibilities to introduce new models, look into the time evolution of quantum system etc.

In this work, we intend not only to provide an outline of relativistic and quasi-Hermitian quantum mechanics but also to show how the theory of quasi-Hermitian operators can be applied in deeper exploration of Klein-Gordon equation.

The first chapter serves as a historical background of development of relativistic quantum mechanics. We review the relativistic wave equations for arbitrary spin and therefore familiarize the reader with the known facts.

The second chapter acquaints the reader with the crypto-Hermitian interpretation of quantum mechanics, in some literature refered to as quasi-Hermitian quantum mechanics [42] or $\mathcal{PT}$-symmetric quantum mechanics [4]. Mathematical foundations and principles of this theory are listed and explained on a few examples. We define important concept of metric operator and its relation to the definition of inner product. Using this terminology it is then straightforward to change the inner product on the same underlying vector space V.

The third chapter is devoted to the problems of proper physical interpretation of Klein-Gordon equation. We introduce Klein-Gordon equation in the Schrödinger form as a useful formalism in its further exploration. Hamiltonian of the Schrödinger form of the Klein-Gordon equation is manifestly non-Hermitian. That is where crypto-Hermitian approach can be applied. We deal with its eigenvalue problem and reconstruct the metric operator for the case of free particle.

The ambitious subject of a correct description of time evolution in quasi-Hermitian quantum mechanics is treated in chapter four. We investigate not only the conditions of quasi-unitarity but also the occurrence of time-dependence in metric operator. Consistent theory of time evolution of quantum system with time-dependent metric operator is presented and illustrated on a few examples.

Possible application of the theory to a broad class of differential models is being shown in the last chapter. 1/L perturbation method is explained and subsequently applied to solvable as well as non solvable models. We obtain a heuristic numerical support of the reality of their spectrum, which is a fundamental condition of applicability of the crypto-Hermitian theory. Because the leading-order terms of the spectrum consists of positive numbers, we can treat the eigenvalues of Klein-Gordon equation as energies.

Some further mathematical aspects of spectral properties of crypto-Hermitian operators are listed in appendixes A and B.

Proper interpretation of Klein-Gordon equation is an important subject, not only because it has direct physical application e.g. in models with pionic atom, but also for the promising connection with several other branches of particle and theoretical physics as we can see e.g. in works of Ali Mostafazadeh [42, 39]. From the broad area of possible exploration and further applications, we narrowed our attention mainly to proper mathematical introduction of the problem, its solution in the discrete case and the possible application of perturbation theory.

Chapter 1

Relativistic quantum mechanics

In order to provide satisfactory description of relativistic quantum object and therefore unite quantum mechanics and special theory of relativity, we need to find proper relativistic wave equation. In this chapter we provide an outline of relativistic wave equations for nonzero mass particles of arbitrary spin.

1.1 Klein-Gordon equation

From historical background can be seen, that the first relativistic wave equation was introduced in 1926 simultaneously by Klein [34], Gordon [27], Kudar [36], Fock [21][22] and de Donder and Van Dungen [13]. Schrödinger himself formulated it earlier in his notes together with the Schrödinger equation [51].

In what follows, we outline the derivation of Klein-Gordon equation as a generalization of Schrödinger equation. For proper mathematical derivation of these equations from first principles see [29]. Schrödinger equation of free particle can be derived from the energy-momentum relation

$$E = \frac{p^2}{2m} \ . \tag{1.1}$$

By the use of a correspondence principle $p \mapsto -i\hbar\nabla$, $E \mapsto i\hbar\partial_t$ we obtain the well known Schrödinger equation

$$i\hbar\partial_t\psi(t,x) = -\frac{\hbar^2}{2m}\nabla^2\psi(t,x) \ . \tag{1.2}$$

Now we repeat the same procedure with relativistic analogue of the energy-momentum relation $E^2 = p^2 + \frac{m^2c^2}{\hbar^2}$. The correspondence principle leads us to Klein-Gordon equation

$$(\Box + \frac{m^2c^2}{\hbar^2})\psi(t,x) = 0 \ , \tag{1.3}$$

where $\Box = \frac{1}{c^2}\partial_t^2 - \Delta = \partial_\mu\partial^\mu$ is the d'Alembert operator. From now on we will use the natural units $c = \hbar = 1$, furthermore we can denote $K = -\Delta + m^2$ and rewrite (1.3) as

$$(i\partial_t)^2\psi(t,x) = K\psi(t,x) \ . \tag{1.4}$$

Unlike Schrödinger equation, the free Klein-Gordon equation is invariant under Lorentz transformation, thus it is an eligible candidate for relativistic quantum mechanical equation. Unfortunately it has other deficiencies which complicate its proper physical interpretation.

There are three fundamental problems arising with the formulation of Klein-Gordon equation. Firstly, for given $\vec{p}$ it allows solutions with both positive and negative energy. For free particles, solution can be found in the form of plane-wave solutions

$$\psi_{\vec{p}}(x,t) = N_{\vec{p}}e^{i(\vec{p}\vec{x}-E(\vec{p})t)} \ , \tag{1.5}$$

where $N_{\vec{p}}$ stands for a normalization constant. If we put this solution into equation (1.3) we obtain energies $E = \pm\sqrt{p^2+m^2}$. This is not a problem for free particles without interaction, because free particle in a positive energy state, stays in positive energy state [45]. "Unphysical" solutions with negative energies are usually reinterpreted as antiparticles.

Secondly, the equation involves second as well as first time derivatives. This means, that in order to solve equation for some ψ at $t > 0$, we need to know both ψ and $\partial_t\psi$ at $t = 0$. In contrast to Schrödinger equation, Klein-Gordon equation has an extra degree of freedom.

Finally, there is a problem with probability interpretation. Proper probability interpretation of the Klein-Gordon equation and its applications to variety of models will be the main topic of this work.

1.2 Dirac equation

In effort to overcome the problems with negative probability densities of the Klein-Gordon equation, Dirac [16] discovered in 1928 another relativistic equation, now named after him. His idea was to avoid time derivatives in the expression for ρ. This can be achieved only if the wave equation doesn't contain higher than first-order time derivatives. Also, in order to satisfy the requirement of relativistic covariance and thus complete symmetry in the treatment of spatial and time components, he was searching for first-order linear differential equation in all four coordinates [52]

$$\partial_t \psi + (\alpha \nabla)\psi + im\beta\psi = 0 \ , \tag{1.6}$$

where $\alpha = (\alpha^1, \alpha^2, \alpha^3)$ and β are constant $N \times N$ Hermitian matrices, $\psi = (\psi_i)$ is $n \times 1$ column matrix of which each component ψ_i, $i = 1, 2 \ldots N$ satisfies the Klein-Gordon equation. That imposes following conditions on α and β

$$\frac{1}{2}(\alpha^i \alpha^j + \alpha^j \alpha^i) = \delta^{ij} \ , \tag{1.7}$$

$$\alpha^i \beta + \beta \alpha^i = 0 \ , \tag{1.8}$$

$$(\alpha^i)^2 = \beta^2 = I \ . \tag{1.9}$$

It also holds, that Trα^i =Tr$\beta = 0$. The dimension N of the explicit representation of the αs and βs must be even. For our special case that $N = 4$ we have

$$\alpha^i = \begin{pmatrix} 0 & \sigma^i \\ \sigma^i & 0 \end{pmatrix} \ , \quad \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \ . \tag{1.10}$$

By denoting $\gamma^0 = \beta$ and $\gamma^i = \beta\alpha^i$ we can rewrite the general form of Dirac equation (1.6) to more convenient form

$$(i\gamma^\mu \partial_\mu - m)\psi = 0 \ . \tag{1.11}$$

Any solution of the Dirac equation automatically solves the Klein-Gordon equation. It can be seen from the decomposition of the Klein-Gordon equation

$$(\Box + m^2)\psi = -(i\gamma^\mu \partial_\mu + m)(i\gamma^\mu \partial_\mu - m)\psi = 0 \ . \tag{1.12}$$

The converse is not true.

Dirac equation describes all spin 1/2 massive particles such as electrons and quarks. Hence, these applications also offer an additional motivation for a deeper study of its Klein-Gordon descendant (1.12).

1.3 Wave equations describing particles with higher spin

Wave equation for relativistic bosons with spin 1 was derived by Proca [47] in 1936

$$\partial_\mu(\partial^\mu A^\nu - \partial^\nu A^\mu) + m^2 A^\nu = 0 \ , \tag{1.13}$$

where A^ν is space-like 4-vector. It can be rewritten in more transparent form as

$$(m^2 - \Box)A_\mu = 0, \quad \partial_\nu A^\nu = 0 \ . \tag{1.14}$$

Note that Proca equation has also been studied in crypto-Hermitian approach in [32].

In 1941 Rarita-Schwinger equation [48] was derived for fermions with spin 3/2. For wave function $\psi_{\mu a}$ the evolution equation would be

$$i\sum_b \gamma_{ab}\partial\psi_{\mu b} - m\psi_{\mu a} = 0 \tag{1.15}$$

with one of the (for solutions of previous equation) equivalent conditions

$$\sum_\mu g_{\mu\mu}\partial_\mu\psi_{\mu a} = 0, \quad \sum_\mu g_{\mu\mu}\gamma_\mu\psi_\mu = 0 \ . \tag{1.16}$$

Elementary particles with spins 3/2 and higher have not been found in nature. Theoretical particle with spin 3/2 is typically called gravitino.

Rarita-Schwinger equation can be generalized [54] for fermions of spin $n+1/2$, where n is an integer. They can be described by wave function $\psi_{\{\mu_1\ldots\mu_n\}a}$, where $\{\mu_1\ldots\mu_n\}$ denotes the symmetrization of the indices $\mu_1,\ldots,\mu_n$, satisfying the evolution equation

$$(i\gamma^\mu\partial_\mu - m)\psi_{\{\mu_1\ldots\mu_n\}a} = 0 \tag{1.17}$$

with supplementary conditions

$$\sum g_{\mu_j\mu_j}\partial_{\mu_j}\psi_{\{\mu_1\ldots\mu_n\}a} = 0 \ , \tag{1.18}$$

$$\sum g_{\mu_j\mu_j}\gamma_{\mu_j}\psi_{\{\mu_1\ldots\mu_n\}a} = 0 \ . \tag{1.19}$$

As was shown in 1948 [3], we can derive a wave function of free particles with arbitrary spin j from Bargmann-Wigner equations

$$(-\gamma^\mu\partial_\mu + m)_{\alpha_r\alpha_r'}\psi_{\alpha_1\ldots\alpha_r'\ldots\alpha_{2j}} = 0 \ , \tag{1.20}$$

where $r = 1, 2, \ldots, 2j$ and ψ is a rank-$2j$ 4-component spinor.

The Rarita-Schwinger and the Bargmann-Wigner wave functions are equivalent, for the same value of the spin.

Chapter 2

Quasi-Hermitian quantum mechanics

One of the axioms of quantum mechanics narrows the class of linear operators, eligible to be identified with observables, to self-adjoint operators only. In following text we give an overview of quasi-Hermitian quantum theory, which broadens the class of such operators to quasi or crypto-Hermitian[1].

Although the underlying ideas date back to the mathematical studies by Dieudonné [15] and to the innovative methodical proposals by Dyson [17], the quasi-Hermitian approach was first formulated as mathematically consistent and widely applicable in the context of nuclear physics in 1992 by Scholtz, Geyer and Hahne [50]. Beyond the realm of nuclear physics the idea has been made extremely popular in 1998 by Bender and Boettcher [5], who introduced infinite class of complex Hamiltonians whose spectra are real and positive

$$H = p^2 + m^2x^2 - (ix)^N \ . \tag{2.1}$$

This started a fast growth of interest in this subject lasting till present day.

[1] Because the concept of quasi-Hermiticity means that the Hermiticity is hidden, or in disguise, in this work we prefer the name crypto-Hermitian as introduced in [31].

2.1 Mathematical background of quantum mechanics

Definition 1. Let A be a linear, densely-defined operator on Hilbert space $\mathcal{H}$. We define *adjoint operator* $A^\dagger$ of A by $\langle\psi|A\varphi\rangle = \langle A^\dagger\varphi|\psi\rangle$ for every φ for which $A^\dagger\varphi$ exists. Adjoint operator is also called *Hermitian conjugate of* A.

Definition 2. Linear, densely-defined operator A is called *self-adjoint*, or *Hermitian*[2] iff $A^\dagger = A$ and $D(A^\dagger) = D(A)$.

Hermitian operators are crucial in formulation of quantum mechanics for several reasons. One of the well known argument is reality of their spectrum, which ensures reality of the readings. Another reason comes from the fact that definition 2 is equivalent to

$$\langle\psi|A\varphi\rangle = \langle A\varphi|\psi\rangle \tag{2.2}$$

for all $\psi, \varphi \in D(A)$. This means that expectation value $\langle\psi|A\psi\rangle$ is real-valued iff A is Hermitian operator. This shows that even though some non-Hermitian operators have real spectrum, observable in quantum mechanics must be chosen from among Hermitian operators.

It is essential to realize that a Hermitian operator can be represented by a non-Hermitian matrix in a nonorthonormal basis. This implies that having the expression for the matrix representation of an operator and knowing the basis used for this representation are not sufficient to decide if the operator is Hermitian. One must in addition know the inner product and be able to determine if the basis is orthonormal [42].

Example 1. Let us consider operator $A : \mathbb{C}^2 \mapsto \mathbb{C}^2$ defined by

$$A\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix} = \begin{pmatrix}-\psi_1-\psi_2\\ \psi_2\end{pmatrix} . \tag{2.3}$$

We can represent this operator in arbitrary basis of $\mathbb{C}^2$. In the standard basis $\mathcal{B}_0$ our operator takes form of a non-Hermitian matrix $A_{\mathcal{B}_0} \neq A^\dagger_{\mathcal{B}_0}$

$$\mathcal{B}_0 = \left\{\begin{pmatrix}1\\0\end{pmatrix}, \begin{pmatrix}0\\1\end{pmatrix}\right\} , \quad A_{\mathcal{B}_0} = \begin{pmatrix}-1 & -1\\ 0 & 1\end{pmatrix} \tag{2.4}$$

[2]In literature regarding crypto-Hermitian quantum mechanics terms "Hermitian" and "self-adjoint" are interchangeable. Although in some mathematical literature, for example [30], is term Hermitian reserved for wider class of operators fulfilling weaker conditions $D(A) \subseteq D(A^\dagger)$, $A^\dagger = A$ on $D(A)$. In this work, we will treat these terms as equivalent within the meaning of definition 2.

and therefore it seems to be apparently non-Hermitian. But we can also represent it in another basis $\mathcal{B}$, in which it takes form of Hermitian matrix $A_{\mathcal{B}} = A_{\mathcal{B}}^{\dagger}$

$$\mathcal{B} = \left\{ \begin{pmatrix} -1 \\ 1 \end{pmatrix}, \begin{pmatrix} 0 \\ -1 \end{pmatrix} \right\} , \quad A_{\mathcal{B}} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} . \tag{2.5}$$

To determine if operator A is Hermitian or not, we need to define inner product on the vector space $\mathbb{C}^2$. If we choose inner product that renders basis $\mathcal{B}_0$ orthonormal, which is the standard Euclidean inner product

$$\langle\psi|\varphi\rangle = \overline{\psi_1}\varphi_1 + \overline{\psi_2}\varphi_2 , \tag{2.6}$$

operator A would be non-Hermitian. On the other hand, if we establish inner product via (A.1) to be

$$\langle\langle\psi|\varphi\rangle = \overline{\psi_1}(2\varphi_1 + \varphi_2) + \overline{\psi_2}(\varphi_1 + \varphi_2) , \tag{2.7}$$

operator A becomes Hermitian. Basis $\mathcal{B}$ is orthonormal with respect to the inner product (2.7).

2.2 Unitary equivalence and modified inner product

Definition 3. Two Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$ are *isomorphic* iff there exist linear surjective map $U : \mathcal{H}_1 \mapsto \mathcal{H}_2$, such that:

$$\langle\psi|\varphi\rangle_1 = \langle U\psi|U\varphi\rangle , \tag{2.8}$$

for all $\psi, \varphi \in \mathcal{H}$.

Theorem 1. [30] Hilbert spaces $\mathcal{H}_1$, $\mathcal{H}_2$ are isomorphic iff $\dim\mathcal{H}_1 = \dim\mathcal{H}_2$.

In particular, any orthonormal set in a separable Hilbert space $\mathcal{H}$ is at most countable [30]. This means that all the infinite-dimensional separable Hilbert spaces are unitarily-equivalent and for instance "friendly" space ℓ_2 represents its canonical realization.

Finite N-dimensional Hilbert spaces are isomorphic to $\mathbb{C}^N$, infinite-dimensional Hilbert spaces are isomorphic to ℓ_2. Unitary equivalence is mediated by unitary operator $U : \mathcal{H} \mapsto \mathbb{C}^N$ for $\dim\mathcal{H} = N < \infty$, or $U : \mathcal{H} \mapsto \ell_2$ for $\dim\mathcal{H} = \infty$

$$U(\psi) := \{\langle\xi_n|\psi\rangle\} , \tag{2.9}$$

where $\psi \in \mathcal{H}$, $\{\xi_n\}$ is orthonormal basis of $\mathcal{H}$ and $\langle \cdot | \cdot \rangle$ is inner product in $\mathcal{H}$.

Therefore, in the choice of the representation of the Hilbert space of states standard quantum mechanics often restricts its attention to the most accessible representations such as ℓ_2 or $L^2(\mathbb{R})$. We shall denote the usually chosen friendly representation of the abstract Hilbert space of states as $\mathcal{H}^{(F)}$.

Definition 4. Let a linear operator $\Theta : \mathcal{H} \mapsto \mathcal{H}$ satisfy following conditions

- Θ is Hermitian, $\Theta = \Theta^\dagger$
- Θ is positive definite, $\langle \varphi | \Theta \varphi \rangle > 0$ for $\forall \varphi \in \mathcal{H}$, $\varphi \neq 0$,
- Θ is everywhere defined[3], $D(\Theta) = \mathcal{H}$.

Than we call such operator *metric* or *metric operator*.

It's shown in appendix A of [50] that positive definiteness of Θ imply its invertibility, bijectivity and boundedness of its inverse. Moreover Hellinger-Toeplitz theorem [49] guarantees its boundedness, because every Hermitian operator defined on entire space $\mathcal{H}$ is bounded.

Consider two Hilbert spaces $\mathcal{H}^{(F)} = (V, \langle \cdot | \cdot \rangle)$, $\mathcal{H}^{(S)} = (V, \langle\langle \cdot | \cdot \rangle)$ defined on the same underlying vector space V, but equipped with two different inner products $\langle \cdot | \cdot \rangle$ and $\langle\langle \cdot | \cdot \rangle$. Inner product $\langle\langle \cdot | \cdot \rangle$ can be obtained from inner product $\langle \cdot | \cdot \rangle$ by means of metric operator in following way

$$\langle\langle \varphi | \psi \rangle = \langle \varphi | \Theta | \psi \rangle \ . \tag{2.10}$$

As was emphasized in [35], boundedness of metric operator Θ is very important property, it guarantees that convergence of Cauchy sequences is not affected by the introduction of new inner product (2.10).

We have one vector space endowed with two different inner products which define Hilbert spaces $\mathcal{H}^{(F)}$ and $\mathcal{H}^{(S)}$. This means we also have two different Hermitian conjugations defining the appropriate dual spaces. Inside the first Hilbert space $\mathcal{H}^{(F)}$ remains the usual Dirac conjugation

$$(|\psi\rangle)^\dagger = \langle \psi | \ . \tag{2.11}$$

[3]Alternatively, we can relax the requirement of "everywhere defined" to "densely defined", but than we need to add requirements of boundedness and bounded inverse. The possibility of the use of unbounded metrics is treated in the last chapter of [2].

Inside the second Hilbert space $\mathcal{H}^{(S)}$, we will use following notation

$$(|\psi\rangle)^\ddagger = \langle\langle\psi| = \langle\psi|\Theta \ , \quad (\langle\langle\psi|)^\ddagger = (\langle\psi|\Theta)^\ddagger = |\psi\rangle. \tag{2.12}$$

Although, for given Hamiltonian H the underlying vector space of the Hilbert space of states is fixed, we still have freedom in our choice of inner product. By defining new inner product we may in some cases find representation $\mathcal{H}^{(S)}$, where the Hamiltonian H becomes self-adjoint. Such representation doesn't exist for arbitrary Hamiltonian H but only for so called "crypto-self-adjoint operators", as defined bellow.

The shift from unphysical but friendly first Hilbert space $\mathcal{H}^{(F)}$ to secondary Hilbert space $\mathcal{H}^{(S)}$ lies in the change of metric operator Θ defining the inner product. In $\mathcal{H}^{(F)}$ we conventionally define the metric operator as trivial $\Theta = 1$. In other words, we introduce $\Theta \neq I$ and, thereby, can work with $\mathcal{H}^{(S)}$as represented in $\mathcal{H}^{(F)}$.

Definition 5. Linear operator $H : \mathcal{H}^{(F)} \mapsto \mathcal{H}^{(F)}$ is called *crypto-Hermitian* or *crypto-self-adjoint* iff there exists metric operator Θ generating inner product, i.e. representation space $\mathcal{H}^{(S)}$, under which is H Hermitian.

Finding proper metric operator Θ for given Hamiltonian H and thus defining new inner product in $\mathcal{H}^{(S)}$ belongs to fundamental problems of crypto-Hermitian quantum mechanic. Often it is very complicated. There are several ways to perform the construction. One of them is to solve *Dieudonné equation* [15]

$$H^\dagger\Theta = \Theta H \ , \tag{2.13}$$

which can be easily obtained by the use of definition 5

$$\langle\psi|\Theta H\varphi\rangle = \langle\langle\psi|H\varphi\rangle = \langle\langle H\psi|\varphi\rangle = \langle H\psi|\Theta\varphi\rangle = \langle\psi|H^\dagger\Theta\varphi\rangle \ . \tag{2.14}$$

Another option used in this work is summation of spectral resolution series, as explained in Appendix B.

2.3 Three-Hilbert-space formulation of quantum mechanics

The concept of crypto-self-adjoint operators is well understandable in the framework of triplet of Hilbert spaces $\mathcal{H}^{(F)}$, $\mathcal{H}^{(S)}$, $\mathcal{H}^{(P)}$as introduced in [61].

The crypto-self-adjointness of an operator can be written in $\mathcal{H}^{(F)}$ as

$$H^\dagger = \Theta H \Theta^{-1} \ . \tag{2.15}$$

In the space $\mathcal{H}^{(S)}$ our crypto-self-adjoint operator becomes self-adjoint in respect to new inner product

$$H^\ddagger = H \ . \tag{2.16}$$

Introduction of third Hilbert space $\mathcal{H}^{(P)}$is linked to another important property of crypto-self-adjoint operator. It is similar to a self-adjoint operator h

$$h = \Omega H \Omega^{-1} = (\Omega H \Omega^{-1})^\dagger = h^\dagger \ . \tag{2.17}$$

This relation can be obtained from decomposition $\Theta = \Omega^\dagger \Omega$ in Dieudonné equation (2.13). Where Ω is an invertible similarity operator, often called Dyson's mapping [17].

Operator h acts on its own representation of the Hilbert space of states denoted by $\mathcal{H}^{(P)}$, we will denote its vectors by spiked kets $|\psi\succ \in \mathcal{H}^{(P)}$. In this representation inner product and Hermitian conjugation of vectors are back to normal, $\Theta = 1$. This physical space is fully consistent with standard textbook quantum mechanics, h is a legitimate quantum observable.

In practical applications of the theory the calculations in $\mathcal{H}^{(P)}$are truly complicated and often practically impossible. Here comes the great benefit of crypto-Hermitian quantum mechanics. Operators h and H are obviously isospectral as far as similarity operator Ω stays bounded, hence we can work with simple non-self-adjoint model with real spectrum and later find its corresponding self-adjoint observable. Another option is to go the other way around, we can map complicated self-adjoint operator h to crypto-Hermitian operator $H \neq H^\dagger$ and make use of much friendlier computing in $\mathcal{H}^{(F)}$, as was done e.g. in nuclear physics application [50].

Three-Hilbert-space formulation of quantum mechanics and properties of particular representation spaces are summarized in table 2.1.

Example 2. We can demonstrate the three Hilbert space formulation of quantum mechanics on our example 1. In case of the matrix representation $A_{\mathcal{B}_0}$ our operator A is represented in the friendly Hilbert space with the well known Euclidean inner product $\mathcal{H}^{(F)} = (\mathbb{C}^2, \langle\cdot|\cdot\rangle)$. Operator acting in more sophisticated secondary Hilbert space $\mathcal{H}^{(S)} = (\mathbb{C}^2, \langle\langle\cdot|\cdot\rangle)$ is represented by

Hilbert space	ket	bra	norm squared
$\mathcal{H}^{(F)}$	$\vert\psi\rangle$	$\langle\psi\vert$	$\langle\psi\vert\psi\rangle$
$\mathcal{H}^{(S)}$	$\vert\psi\rangle$	$\langle\langle\psi\vert = \langle\psi\vert\Theta$	$\langle\langle\psi\vert\psi\rangle = \langle\psi\vert\Theta\vert\psi\rangle$
$\mathcal{H}^{(P)}$	$\vert\psi\succ = \Omega\vert\psi\rangle$	$\prec\psi\vert = \langle\psi\vert\Omega^\dagger$	$\prec\psi\vert\psi\succ = \langle\psi\vert\Theta\vert\psi\rangle$

Table 2.1: Three-Hilbert-space formulation notation

the matrix $A_{\mathcal{B}}$. Inner product in $\mathcal{H}^{(S)}$ expressed by (2.7) is determined by metric operator

$$\Theta = \begin{pmatrix} 2 & 1 \\ 1 & 1 \end{pmatrix} . \tag{2.18}$$

That can be decomposed by means of Dyson's mapping Ω, $\Theta = \Omega^\dagger\Omega$. One of the possible decompositions is

$$\Theta = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix} . \tag{2.19}$$

Now we can reconstruct the one of the isospectral operators $a = \Omega A \Omega^{-1}$

$$a = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix} . \tag{2.20}$$

Operator a acts in physical Hilbert space $\mathcal{H}^{(P)}$ in which it is Hermitian with respect to the standard Euclidean inner product. All the vectors including the basis are mapped by Dyson's map $|\psi\succ = \Omega|\psi\rangle$ to the new vector space, which in this particular example coincides with the old one $\mathcal{H}^{(P)} = (\mathbb{C}^2, \langle\cdot|\cdot\rangle)$.

Note that for given crypto-Hermitian operator A, isospectral operator a is not uniquely defined. It depends on the particular choice of metric Θ and Dyson's mapping Ω.

2.4 One-parametric model in two dimensions

Let us consider crypto-Hermitian Hamiltonian with parameter $a \in \mathbb{R}$ in the form of matrix 2×2

$$H = \begin{pmatrix} -1 & a \\ -a & 1 \end{pmatrix} . \tag{2.21}$$

Solving the equation $H\psi = \lambda\psi$ we find its eigenvalues and eigenvectors

$$\lambda_{1/2} = \pm\sqrt{1-a^2} \ , \ \psi_{1/2} = \begin{pmatrix} a \\ -1 \pm \sqrt{1-a^2} \end{pmatrix} . \tag{2.22}$$

We can see that the eigenvalues of our operator are real for parameter $a \in \langle -1, 1 \rangle$.

Under this condition we can calculate exact form of metric operator Θ from Dieudonné equation $H^\dagger \Theta = \Theta H$. Together with conditions of positivity and Hermiticity that we put upon Θ we obtain two-parametric family of metrics

$$\theta(\alpha, \beta) = \begin{pmatrix} \alpha & \frac{-a(\alpha+\beta)}{2} \\ \frac{-a(\alpha+\beta)}{2} & \beta \end{pmatrix} , \tag{2.23}$$

where α and β satisfy following conditions

$$\alpha > 0,\ \beta \in (\beta_1,\ \beta_2)\ ,\ \beta_{1/2} = \alpha \left[-1 + \frac{2}{a^2}(1 \pm \sqrt{1-a^2}) \right] . \tag{2.24}$$

Now, we construct Dyson's map Ω. From the broad class of possible decomposition we choose to prefer the most easily invertible triangular-matrix form. Thus, with the help of Cholesky decomposition method we have

$$\Omega(\alpha, \beta) = \begin{pmatrix} \sqrt{\alpha} & 0 \\ -\frac{a(\alpha+\beta)}{2\sqrt{\alpha}} & \sqrt{\beta - \frac{a^2(\alpha+\beta)^2}{4\alpha}} \end{pmatrix} , \tag{2.25}$$

which leads us to family of isospectral operators h acting in $\mathcal{H}^{(P)}$

$$h(\alpha, \beta) = \begin{pmatrix} -1 + \frac{a^2(\alpha+\beta)}{2\alpha} & -\frac{a}{\sqrt{\alpha}}\sqrt{\beta - \frac{a^2(\alpha+\beta)^2}{4\alpha}} \\ -\frac{a}{\sqrt{\alpha}}\sqrt{\beta - \frac{a^2(\alpha+\beta)^2}{4\alpha}} & -1 + \frac{a^2(\alpha+\beta)}{2\alpha} \end{pmatrix} . \tag{2.26}$$

Their eigenvectors are related to the original eigenvector of H by $|\psi_{1/2} \succ = \Omega|\psi_{1/2}\rangle$

$$|\psi_{1/2} \succ = \begin{pmatrix} -\frac{(-1\pm\sqrt{1-a^2})\sqrt{\alpha}}{a} - \frac{a(\alpha+\beta)}{2\sqrt{\alpha}} \\ \sqrt{\beta - \frac{a^2(\alpha+\beta)^2}{4\alpha}} \end{pmatrix} . \tag{2.27}$$

This example nicely illustrates the characteristic contrast between the simple form of H and much less friendly, complicated form of h.

Chapter 3

Probability interpretation of Klein-Gordon equation

The problem of proper probability interpretation of Klein-Gordon equation is old, as the equation itself. As we can study in almost every textbook on relativistic quantum theory [28, 45, 10], it requires definition of non-negative, integrable function $\rho(t,x) = j^0(t,x)$ called *probability density*, which satisfies the continuity equation

$$\nabla_\mu j^\mu = 0 \ . \tag{3.1}$$

By simple operating with the Klein-Gordon equation

$$\psi^*(\Box + m^2)\psi - \psi(\Box + m^2)\psi^* = 0 = \nabla_\mu j^\mu \tag{3.2}$$

we obtain possible form of a *four-current* $j^\mu = (\rho, \vec{j}\,)$

$$j^\mu(t,x) = \frac{i}{2m}(\psi^*\partial^\mu\psi - \psi\partial^\mu\psi^*). \tag{3.3}$$

Note that the *current* $\vec{j}$ is the same as in the case of Schrödinger equation, however the density is not $\rho_{KG} \neq \rho_S = \psi^*\psi$,

$$\rho_{KG} = \frac{i}{2m}(\psi^*\partial_t\psi - \psi\partial_t\psi^*) \ . \tag{3.4}$$

By inserting the stationary states $i\partial_t\psi = E\psi$ and $-i\partial_t\psi^* = E\psi^*$ into the expression (3.4), we can investigate the behavior of the density function ρ

$$\rho = \frac{E}{m}\psi^*\psi \ . \tag{3.5}$$

In the non-relativistic limit, we find that the density function of the Klein-Gordon equation coincides with the density function of the Schrödinger equation, $\rho_S = \rho_{KG}$. Although in the relativistic case, energy can be both positive and negative, therefore ρ_{KG} is indefinite and it cannot by consistently interpreted as a probability density.

Corresponding Klein-Gordon inner product

$$\langle\varphi|\psi\rangle_{KG} = \frac{i}{2m}(\langle\varphi|\partial^t\psi\rangle - \langle\partial^t\varphi|\psi\rangle) , \tag{3.6}$$

is also indefinite.

Following alternative, originated in the work of Pauli and Weisskopf [46], is often used. If we reinterpret Klein-Gordon equation as a field equation satisfied by a quantum field $\psi(x)$, and multiply (3.4) by elementary charge e we can obtain *charge density operator* describing a Klein-Gordon field of charged particles

$$\rho(t,x) = \frac{ie}{2m}(\psi^*\partial_t\psi - \psi\partial_t\psi^*) , \tag{3.7}$$

for further reference see e.g. [28, 45, 53]. In our work we abandon this concept and investigate an option of finding non-negative density function by means of redefinition of the inner product and the concept of crypto-Hermitian quantum theory.

3.1 Schrödinger form of Klein-Gordon equation

The fact that Klein-Gordon equation is differential equation of second order in time gives it an extra degree of freedom. Feshbach and Villars [20] suggested solution to this problem by introducing two-component wave function and therefore making the extra degree of freedom more visible. Following their ideas together with even earlier ideas of Foldy [23], we can replace Klein-Gordon equation with two differential equation of first order in time. Inspired by convention introduced in [56] we put

$$\Psi^{(1)} = i\partial_t\psi , \quad \Psi^{(2)} = \psi . \tag{3.8}$$

Now, equation (1.4) can be decomposed into a pair of partial differential equations

$$i\partial_t \Psi^{(1)} = K\Psi^{(2)} \ , \tag{3.9}$$
$$i\partial_t \Psi^{(2)} = \Psi^{(1)} \ , \tag{3.10}$$

which, written in the matrix form, become

$$i\partial_t \begin{pmatrix} \Psi^{(1)} \\ \Psi^{(2)} \end{pmatrix} = \begin{pmatrix} 0 & K \\ I & 0 \end{pmatrix} \begin{pmatrix} \Psi^{(1)} \\ \Psi^{(2)} \end{pmatrix} \ . \tag{3.11}$$

Hamiltonian of the quantum system takes form

$$H = \begin{pmatrix} 0 & K \\ 1 & 0 \end{pmatrix} \ , \tag{3.12}$$

and enters the Schrödinger equation

$$i\partial_t \Psi(t,x) = H\Psi(t,x) \ , \quad \Psi = \begin{pmatrix} \Psi^{(1)} \\ \Psi^{(2)} \end{pmatrix} \ . \tag{3.13}$$

Two-component vectors $\Psi(t)$ belong to

$$\mathcal{H} = L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3) \tag{3.14}$$

and the Hamiltonian H may be viewed as acting in $\mathcal{H}$.

The so called Schrödinger form of Klein-Gordon equation (3.13) is equivalent to the original Klein-Gordon equation (1.3). It is in more familiar form, although, new challenge arises with the manifest non-Hermiticity of Hamiltonian (3.12). Equation (3.13) must be treated in the quasi-Hermitian framework, as described in chapter 2. The probability density function, necessary to its proper probability interpretation, must be defined by means of a new metric dependent inner product defining another Hilbert space $\mathcal{H}^{(S)}$.

Remark 1. In the related literature, such as [39], [20] or [28], different decomposition into two first order differential equation is being used to get the Schrödinger form of the Klein-Gordon equation

$$i\partial_t \varphi = -\frac{1}{2m}\Delta(\varphi + \chi) + m\varphi \ , \tag{3.15}$$
$$i\partial_t \chi = \frac{1}{2m}\Delta(\varphi + \chi) - m\chi \ , \tag{3.16}$$

where we put $\psi = \varphi + \chi$ and $i\partial_t\psi = m(\varphi - \chi)$. The new variables φ, χ may be expressed via the wavefunction ψ as

$$\varphi = \frac{1}{2}\left(\psi + \frac{i}{m}\partial_t\psi\right) \ , \quad \chi = \frac{1}{2}\left(\psi - \frac{i}{m}\partial_t\psi\right) \ . \tag{3.17}$$

This form of decomposition is convenient mainly because the non-relativistic limit is well visible. For free particle of positive energy at rest we have (lets remember we put $c^2 = 1$ in the begining)

$$\psi \sim e^{-imt} = \frac{i}{m}\partial_t\psi \ , \tag{3.18}$$

which gives us

$$\chi = 0 \ , \quad \varphi \sim e^{-imt} \ . \tag{3.19}$$

Therefore at non-relativistic velocities χ will be negligible compared to φ and vice versa for negative energy particles.

3.2 The calculation of eigenvalues

New form of Klein-Gordon equation (3.13) have many benefits. One of them is simplification of calculation of its eigenvalues to mere solving the eigenvalue problem for operator K

$$K\psi_n = \epsilon_n\psi_n \ . \tag{3.20}$$

The relationship between eigenvalues ϵ_n of the operator K and eigenvalues E_n of the non-Hermitian operator H of the Schrödinger form of Klein-Gordon equation

$$\begin{pmatrix} 0 & K \\ I & 0 \end{pmatrix} \begin{pmatrix} \Psi^{(1)} \\ \Psi^{(2)} \end{pmatrix} = E \begin{pmatrix} \Psi^{(1)} \\ \Psi^{(2)} \end{pmatrix} \tag{3.21}$$

can be easily seen. Equation (3.21) is formed from two algebraic equations

$$K\Psi^{(2)} = E\Psi^{(1)} \ , \quad \Psi^{(1)} = E\Psi^{(2)} \ . \tag{3.22}$$

After insertion of the second one to the first one we obtain

$$K\Psi^{(2)}_n = E_n^2\Psi^{(2)}_n \ , \tag{3.23}$$

which compared with equation (3.20) gives us following relation between eigenvalues

$$\epsilon_n = E_n^2 \ . \tag{3.24}$$

We can see, that eigenvalues E_n remain real under assumption of $\epsilon_n > 0$. Corresponding eigenvectors

$$H\Psi_n^{(\pm)} = E_n^{(\pm)}\Psi_n^{(\pm)} \ , \quad \Psi_n^{(\pm)} = \begin{pmatrix} \pm\sqrt{\epsilon_n}\psi_n \\ \psi_n \end{pmatrix} \tag{3.25}$$

Example 3 (Free Klein-Gordon equation)**.** Operator

$$K = -\Delta + m^2 \tag{3.26}$$

acting on $\mathcal{H} = L^2(\mathbb{R}^3)$ is positive and Hermitian. It has continuous and degenerate spectrum. As suggested in [38], we identify the space $\mathbb{R}^3$ with the volume of a cube of side l, as l tends to infinity. Than we can treat the continuous spectrum of K as the limit of the discrete spectrum corresponding to the approximation. The eingenvalues are given by

$$\epsilon_{\vec{k}} = k^2 + m^2 \tag{3.27}$$

and corresponding eigenvectors $\psi_{\vec{k}} = \Psi_{\vec{k}}^{(2)}$ are

$$\psi_{\vec{k}}(\vec{x}) = \langle\vec{x}|\vec{k}\rangle = (2\pi)^{-3/2}e^{i\vec{k}.\vec{x}} \ , \tag{3.28}$$

where $\vec{k} \in \mathbb{R}^3$ and $\vec{k}.\vec{k} = k^2$. We can see that $\psi_{\vec{k}} \notin L^2(\mathbb{R}^3)$. They are generalized eigenvectors, i.e. vectors which eventually becomes 0 if $(K - \lambda I)$ is applied to it enough times successively, describing scattering states [38].

Vectors $\psi_{\vec{k}}$ satisfy orthonormality and completeness conditions

$$\langle\vec{k}|\vec{k}'\rangle = \delta(\vec{k} - \vec{k}') \ , \quad \int d^3k|\vec{k}\rangle\langle\vec{k}|) = 1 \tag{3.29}$$

and operator K can be expressed by its spectral resolution as

$$K = \int d^3k(k^2 + m^2)|\vec{k}\rangle\langle\vec{k}| \ . \tag{3.30}$$

From the relations (3.24) and (3.25) we see that eigenvalues and eigenvectors of H are given by

$$E_{\vec{k}}^{(\pm)} = \pm\sqrt{\vec{k}^2 + m^2} \ , \quad \Psi_{\vec{k}}^{(\pm)} = \begin{pmatrix} \pm\sqrt{\vec{k}^2 + m^2} \\ 1 \end{pmatrix} \psi_{\vec{k}} \ . \tag{3.31}$$

The eigenvectors $\Phi_{\vec{k}}^{(\pm)}$ of adjoint operator $H^\dagger$ are

$$\Phi_{\vec{k}}^{(\pm)} = \begin{pmatrix} 1 \\ \pm\sqrt{\vec{k}^2 + m^2} \end{pmatrix} \psi_{\vec{k}} \ , \tag{3.32}$$

which form together with $\Psi^{(\pm)}_{\vec{k}}$ complete biorthogonal system

$$\langle \Phi^{(\nu)}_{\vec{k}'} | \Psi^{(\nu')}_{\vec{k}} \rangle = \delta(\vec{k} - \vec{k}') \delta_{\nu\nu'} 2E^{(\nu)}_{\vec{k}} \ , \tag{3.33}$$

where $\nu, \nu' = \pm 1$.

3.3 Construction of the metric

One of the possible ways how to construct metric operator Θ for given crypto-Hermitian Hamiltonian H is by summing the spectral resolution series (B.9). It requires the solution of eigenvalue problem for $H^\dagger$. In what follows, we try to construct the metric operator for free Klein-Gordon equation

$$\Theta = \int d^3k \left(\alpha^{(+)} |\Phi^{(+)}_{\vec{k}}\rangle \langle \Phi^{(+)}_{\vec{k}}| + \alpha^{(-)} |\Phi^{(-)}_{\vec{k}}\rangle \langle \Phi^{(-)}_{\vec{k}}| \right) \ , \tag{3.34}$$

where we insert eigenvectors $\Phi^{(\pm)}_{\vec{k}}$ as computed in (3.32)

$$\Theta = \int d^3k \begin{pmatrix} (\alpha^{(+)} + \alpha^{(-)}) & (\alpha^{(+)} - \alpha^{(-)})\sqrt{k^2+m^2} \\ (\alpha^{(+)} - \alpha^{(-)})\sqrt{k^2+m^2} & (\alpha^{(+)} + \alpha^{(-)})(k^2+m^2) \end{pmatrix} |\vec{k}\rangle\langle\vec{k}| \ . \tag{3.35}$$

By means of equation (3.30) and by putting

$$K^{1/2} = \int d^3k \sqrt{k^2+m^2} |\vec{k}\rangle\langle\vec{k}| \tag{3.36}$$

we obtain family of metric operators

$$\Theta = \begin{pmatrix} \alpha & \beta K^{1/2} \\ \beta K^{1/2} & \alpha K \end{pmatrix} \ , \tag{3.37}$$

where $\alpha = (\alpha^{(+)} + \alpha^{(-)})$, $\beta = (\alpha^{(+)} - \alpha^{(-)})$.

Unfortunately, the metric operator (3.37) is unbounded and therefore doesn't satisfy all the requested properties we put upon metric operator. Under some conditions similarity operator Ω may still be constructed even in the case of unbounded metric operator. Which can be deeper studied e.g. in [2] or [1].

Still with the knowledge of the metric operator (3.37), we can construct positive definite inner product defining Hilbert space $\mathcal{H}^{(S)}$

$$\langle\langle \Psi | \Phi \rangle = \alpha(\langle \psi | K | \varphi \rangle + \langle \dot{\psi} | \dot{\varphi} \rangle) + i\beta(\langle \psi | K^{1/2} | \dot{\varphi} \rangle - \langle \dot{\psi} | K^{1/2} | \varphi \rangle) \ . \tag{3.38}$$

The integrand of newly found inner product defines probability density

$$\rho(x) = \alpha(\psi^*(x)K\varphi(x) + \dot{\psi}^*(x)\dot{\varphi}(x)) + i\beta(\psi^*(x)K^{1/2}\dot{\varphi}(x) - \dot{\psi}^*(x)K^{1/2}\varphi(x)) \ . \tag{3.39}$$

Complicated problems with locality, defining of physical observables and attempts to construct conserved four-current can be thoroughly studied in further references [43, 44]. The problem becomes much simpler if we narrow our attention to real Klein-Gordon fields only. It was shown that in such a case, inner product is uniquely defined [43, 33]

The next step of this process would be construction of appropriate metric operator for Klein-Gordon equation with nonzero potential V as was done for special cases in [56, 67, 43, 44]. It is also possible to broaden the formalism by adding manifest non-Hermiticity in operator $K \neq K^\dagger$, as was shown in [57].

Chapter 4

The discretization approach

To overcome the problems with unboundedness of metric operator (3.37), we choose to shift our attention to discrete model. In the discrete approximation the metric operator stays bounded and we are able to reconstruct the similar Hermitian Hamiltonians h.

4.1 Discrete model

As was shown in [62], Laplace operator Δ can be discretized into matrix form

$$H^{(N)} = \begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & -1 & 2 & \ddots & \\ & & \ddots & \ddots & -1 \\ & & & -1 & 2 \end{pmatrix} \tag{4.1}$$

Matrix (4.1) is Hermitian and therefore diagonalizable, i.e. similar to diagonal matrix. Hence, in further calculation we will operate with diagonal matrix only.

4.2 Matrix 2×2

First, we will show the procedure on more simple example of Hamiltonian K in the form of 2×2 real symmetric matrix

$$K = \begin{pmatrix} 2 & 0 \\ 0 & 3 \end{pmatrix} . \tag{4.2}$$

Recall that K takes place in the Schrödinger form of Klein-Gordon operator

$$H = \begin{pmatrix} 0 & K \\ I & 0 \end{pmatrix} . \tag{4.3}$$

In order to find metric operator, we put our Hamiltonian into Dieudonné equation (2.13). Together with Hermiticity condition $\Theta^+ = \Theta$, we obtain 4-parametric family of metrics

$$\Theta = \begin{pmatrix} \alpha & 0 & \gamma & 0 \\ 0 & \beta & 0 & \delta \\ \gamma & 0 & 2\alpha & 0 \\ 0 & \delta & 0 & 3\beta \end{pmatrix} . \tag{4.4}$$

Requirement on positive-definitness of the metric put following conditions on our parameters

$$\alpha > 0 \ , \ \beta > 0 \ , \ 2\alpha^2 > \gamma^2 \ , \ 3\beta^2 > \delta^2 \ . \tag{4.5}$$

Now, we can employ Cholesky decomposition method to find proper factorization of the metric $\Theta = \Omega^+\Omega$

$$\Omega = \begin{pmatrix} \sqrt{\alpha} & 0 & \frac{\gamma}{\sqrt{\alpha}} & 0 \\ 0 & \sqrt{\beta} & 0 & \frac{\delta}{\sqrt{\beta}} \\ 0 & 0 & \sqrt{\frac{2\alpha^2-\gamma^2}{\alpha}} & 0 \\ 0 & 0 & 0 & \sqrt{\frac{3\beta^2-\delta^2}{\beta}} \end{pmatrix} . \tag{4.6}$$

Finally, we map non-Hermitian operator H to new physical hermitian operator $h = \Omega H \Omega^{-1}$, $h^+ = h$

$$h = \begin{pmatrix} \frac{\gamma}{\alpha} & 0 & \frac{\sqrt{2\alpha^2-\gamma^2}}{\alpha} & 0 \\ 0 & \frac{\delta}{\beta} & 0 & \frac{\sqrt{3\beta^2-\delta^2}}{\beta} \\ \frac{\sqrt{2\alpha^2-\gamma^2}}{\alpha} & 0 & -\frac{\gamma}{\alpha} & 0 \\ 0 & \frac{\sqrt{3\beta^2-\delta^2}}{\beta} & 0 & -\frac{\delta}{\beta} \end{pmatrix} . \tag{4.7}$$

4.3 Matrix $n \times n$

Now, we generalize this process to $n \times n$ real diagonal matrix, which represents the discrete case of Laplace operator

$$K = \begin{pmatrix} a_1 & 0 & \cdots & 0 \\ 0 & a_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & a_n \end{pmatrix} . \tag{4.8}$$

Let A, B, C be real matrices $n \times n$, where $A = A^T$, $B = B^T$. Than we can write the Dieudonné equation (2.13) by means of block matrices

$$\begin{pmatrix} 0 & I \\ K & 0 \end{pmatrix} \begin{pmatrix} A & C^T \\ C & B \end{pmatrix} = \begin{pmatrix} A & C^T \\ C & B \end{pmatrix} \begin{pmatrix} 0 & K \\ I & 0 \end{pmatrix} . \tag{4.9}$$

We obtain following conditions

$$C = C^T,\ KC = C^T K,\ B = KA = AK . \tag{4.10}$$

Real symmetric matrix which commutes with diagonal matrix must be diagonal. Thus the form of our metric operator is as follows

$$\Theta = \begin{pmatrix} \alpha_1 & \cdots & 0 & \beta_1 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & \alpha_n & 0 & \cdots & \beta_n \\ \beta_1 & \cdots & 0 & a_1\alpha_1 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & \beta_n & 0 & \cdots & a_n\alpha_n \end{pmatrix} . \tag{4.11}$$

It depends on $2n$ parameters $\alpha_1 \ldots \alpha_n$, $\beta_1 \ldots \beta_n$.

We can see the correspondence between discrete metric (4.11) and metric of the continuous case (3.37).

From Cholesky decomposition method we get factorization in triangular matrices $\Theta = \Omega^{+}\Omega$

$$\Omega = \begin{pmatrix} \sqrt{\alpha_1} & \cdots & 0 & \frac{\beta_1}{\sqrt{\alpha_1}} & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & \sqrt{\alpha_n} & 0 & \cdots & \frac{\beta_n}{\sqrt{\alpha_n}} \\ 0 & \cdots & 0 & \sqrt{\frac{a_1\alpha_1^2-\beta_1^2}{\alpha_1}} & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & 0 & \cdots & \sqrt{\frac{a_n\alpha_n^2-\beta_n^2}{\alpha_n}} \end{pmatrix}. \tag{4.12}$$

Finally, the sought form of Hermitian operator $h = h^{\dagger}$, $h = \Omega H \Omega^{-1}$ is

$$h = \begin{pmatrix} \frac{\beta_1}{\alpha_1} & \cdots & 0 & \frac{\sqrt{a_1\alpha_1^2-\beta_1^2}}{\alpha_1} & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & \frac{\beta_n}{\alpha_n} & 0 & \cdots & \frac{\sqrt{a_n\alpha_n^2-\beta_n^2}}{\alpha_n} \\ \frac{\sqrt{a_1\alpha_1^2-\beta_1^2}}{\alpha_1} & \cdots & 0 & -\frac{\beta_1}{\alpha_1} & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & \frac{\sqrt{a_n\alpha_n^2-\beta_n^2}}{\alpha_n} & 0 & \cdots & -\frac{\beta_n}{\alpha_n} \end{pmatrix}. \tag{4.13}$$

New operator h is isospectral to original operator H, in addition, because of its Hermiticity, it is fully compatible with traditional textbook quantum mechanics. Time evolution of states follows Schrödinger equation.

Chapter 5

Time evolution of quantum system

With the knowledge of the initial state $|\varphi(0)\succ$, the problem of time evolution in quantum mechanics is fully described by Schrödinger equation

$$i\partial_t|\varphi(t)\succ = h(t)|\varphi(t)\succ \quad . \tag{5.1}$$

For the most common choices of linear differential Hamiltonian operators it's a partial differential equation the solution of which can be written in form

$$|\varphi(t)\succ = u(t)|\varphi(0)\succ \ , \tag{5.2}$$

where $u(t)$ is a unitary operator called *the evolution operator*. It also satisfies the Schrödinger equation

$$i\partial_t u(t) = h(t)u(t) \ . \tag{5.3}$$

For time independent Hamiltonians $h \neq h(t)$ it takes exponential form

$$u(t) = e^{-iht} \ . \tag{5.4}$$

The postulate of unitarity of the evolution operator $u(t)$ comes from the requirement of norm preservation during the time evolution

$$\prec\varphi(t)|\varphi(t)\succ = \prec\varphi(0)|u^\dagger(t)u(t)|\varphi(0)\succ = \prec\varphi(0)|\varphi(0)\succ \tag{5.5}$$

together with the fact that $u(0) = 1$.

5.1 Quasi-stationary time evolution

It is well known how the time evolution works for self-adjoint operators in Hilbert space $\mathcal{H}^{(P)}$. In what follows we wish to examine what equation determines the time evolution of crypto-self-adjoint operators in representation spaces $\mathcal{H}^{(F)}$ and $\mathcal{H}^{(S)}$ and what role plays in it the metric operator Θ. In order to do so, we map the Schrödinger equation (5.1) acting in the space $\mathcal{H}^{(P)}$ by means of Dyson's map Ω to the friendly space $\mathcal{H}^{(F)}$. It holds that

$$|\varphi(t)\succ = \Omega|\varphi(t)\rangle \ , \quad h(t) = \Omega H(t)\Omega^{-1} \ . \tag{5.6}$$

Lets assume the Dyson's mapping to be time-independent $\Omega \neq \Omega(t)$, therefore implying time-independence of metric operator $\Theta \neq \Theta(t)$. The Schrödinger equation will be in the standard form

$$i\partial_t|\varphi(t)\rangle = H(t)|\varphi(t)\rangle \tag{5.7}$$

except the fact, that operator $H(t)$ is crypto-Hermitian $H^\dagger(t)\Theta = \Theta H(t)$, $\Theta = \Omega^\dagger\Omega$. Therefore the evolution operator solving the equation (5.7) is no longer unitary

$$U(t) = \Omega^{-1}u(t)\Omega \ , \quad U^\dagger(t)U(t) \neq 1 \ , \tag{5.8}$$

specially for time-independent Hamiltonian $h \neq h(t)$ it follows from $H = \Omega^{-1}h\Omega$ that

$$U(t) = e^{-iHt} \ , \quad U^\dagger(t)U(t) = e^{i(H^\dagger - H)t} \neq 1 \ . \tag{5.9}$$

The postulate of unitarity of quantum evolution seems to be broken. But as suggested in [41] we can solve this problem easily by the change of inner product, i.e. shift to the secondary representation space $\mathcal{H}^{(S)}$. It is possible for us to generalize the condition of unitarity of the evolution operator $u(t)$ to the condition of *quasi-unitarity* of operator $U(t)$

$$U^\dagger(t)\Theta U(t) = \Theta \ . \tag{5.10}$$

We can see, that the quasi-unitarity condition naturally arises from the requirement of norm preservation in $\mathcal{H}^{(S)}$

$$\langle\langle\varphi(t)|\varphi(t)\rangle = \langle\varphi(t)|\Theta|\varphi(t)\rangle = \langle\varphi(0)|U^\dagger(t)\Theta U(t)|\varphi(0)\rangle = \langle\varphi(0)|\Theta|\varphi(0)\rangle = \langle\langle\varphi(0)|\varphi(0)\rangle \ . \tag{5.11}$$

As was pointed out in [41], time-independent metric operator of time-dependent crypto-self-adjoint operator

$$H^\dagger(t) = \Theta H(t)\Theta^{-1} \ , \quad \Theta \neq \Theta(t) \tag{5.12}$$

is uniquely defined up to an unimportant multiplicative positive constant.

5.2 The problem of time-dependent metrics

In the previous section, we narrowed our attention to the time-independent metrics only. This concept was properly explained for example in [14, 41]. Subsequently, it was pointed out, that we are able to formulate unitary time evolution even when manifest time-dependency occurs in the metric operator [58, 60, 61]. In such a case Schrödinger equation in $\mathcal{H}^{(F)}$would be in form

$$i\partial_t|\varphi(t)\rangle = [H(t) - i\Omega^{-1}(t)\dot{\Omega}(t)]|\varphi(t)\rangle \ , \tag{5.13}$$

where $\dot{\Omega}(t)$ stands for time derivative of Ω and we made use of relationships

$$|\varphi(t)\succ = \Omega(t)|\varphi(t)\rangle \ , \quad h(t) = \Omega(t)H(t)\Omega^{-1}(t) \ . \tag{5.14}$$

We can see, that crypto-Hermitian operator $H(t)$ no longer generates the time evolution in $\mathcal{H}^{(F)}$and therefore cannot be interpreted as a Hamiltonian any more. The time-evolution is generated by another operator G

$$G(t) = H(t) - \Sigma(t) \ , \quad \Sigma(t) = i\Omega^{-1}(t)\dot{\Omega}(t) \tag{5.15}$$

and its Hermitian conjugate $G^\dagger$. The evolution of states is than described by two Schrödinger equations

$$i\partial_t|\varphi(t)\rangle = G(t)|\varphi(t)\rangle \ , \tag{5.16}$$
$$i\partial_t|\varphi(t)\rangle\rangle = G^\dagger(t)|\varphi(t)\rangle\rangle \ , \tag{5.17}$$

where $|\varphi(t)\rangle\rangle = (\langle\langle\varphi(t)|)^\dagger$. Each of these equations is solved by its own evolution operator, $U_R(t)$ and $U_L^\dagger(t)$

$$|\varphi(t)\rangle = U_R(t)|\varphi(0)\rangle \ , \quad |\varphi(t)\rangle\rangle = U_L^\dagger(t)|\varphi(0)\rangle\rangle \ . \tag{5.18}$$

satisfying corresponding Schrödinger equations

$$i\partial_t U_R(t) = G(t)U_R(t), \tag{5.19}$$
$$i\partial_t U_L^\dagger(t) = G^\dagger(t)U_L^\dagger(t). \tag{5.20}$$

The pair of evolution operators U_L, U_R is obtained from the original evolution operator $u(t)$ in following way

$$U_R(t) = \Omega^{-1}(t)u(t)\Omega(0) \ , \quad U_L^\dagger(t) = \Omega^\dagger(t)u(t)(\Omega^{-1}(0))^\dagger \ . \tag{5.21}$$

It holds that $U_L(t)U_R(t) = 1$ for every $t > 0$, hence the requirement of the norm preservation of evolving state is satisfied

$$\langle\langle\varphi(t)|\varphi(t)\rangle = \langle\langle\varphi(0)|U_L(t)U_R(t)|\varphi(0)\rangle = \langle\langle\varphi(0)|\varphi(0)\rangle \ . \tag{5.22}$$

From the definition of operator $G(t)$ we can easily derive differential equation for the metric

$$i\dot{\Theta} = G^{\dagger}(t)\Theta(t) - \Theta(t)G(t) \ , \tag{5.23}$$

where $\dot{\Theta}$ stands for time derivative of the metric operator. Equation (5.22) shows us another approach to the time evolution of crypto-Hermitian operators and it allows us to reconstruct the metric operator via its direct solution, as was shown in [7, 8]. We can see, that in case $\Theta \neq \Theta(t)$ equation (5.22) coincides with hidden Hermiticity condition (2.13) and operator $G(t)$ becomes crypto-Hermitian.

In order to simplify the search for evolution operators U_L, U_R and the subsequent return to the original physical space $\mathcal{H}^{(P)}$we make an assumption that our choice of $\Omega(t)$ implies time-independence of $G \neq G(t)$. In other words for the generator of time evolution holds $G(t) = G(0)$ for all $t > 0$. Therefore, the time evolution of wave functions $|\varphi(t)\rangle \in \mathcal{H}^{(F)}$and $|\varphi(t)\rangle\rangle \in \mathcal{H}^{(F)}$follows the well known exponential formulas

$$|\varphi(t)\rangle = \exp(-iG(0)t)|\varphi(0)\rangle \ , \quad |\varphi(t)\rangle\rangle = \exp(-iG^{\dagger}(0)t)|\varphi(0)\rangle\rangle \ . \tag{5.24}$$

In [64] a method of construction of such Dyson's mapping $\Omega(t)$ was suggested. It was sufficient to assume the existence of such Ω at initial time $t = 0$ and infinitesimally shifted time $\Delta = 0 + dt > 0$. Operator $G(t) = G(0) = G$ than could be reconstructed via

$$G = \Omega^{-1}(0)h(0)\Omega(0) - i\Omega^{-1}(0)\dot{\Omega}(0) \ , \tag{5.25}$$

where the time derivative of $\Omega(0)$ was approximately determined by

$$\dot{\Omega}(0) \approx \frac{\Omega(\Delta) - \Omega(0)}{\Delta} + \mathcal{O}(\Delta^2) \ . \tag{5.26}$$

The final step of the constructive return to the original Hilbert space $\mathcal{H}^{(P)}$still remains complicated. It requires computation of explicit value of the Dyson's operator $\Omega(t)$ at all times. The above-mentioned assumption of $\partial_t G(t) = \dot{H}(t) + \dot{\Sigma}(t) = 0$ may be rewritten as

$$i\dot{\sigma}(t) = i\dot{h}(t) + h(t)\sigma(t) - \sigma(t)h(t) \ , \tag{5.27}$$

where $\Sigma(t) = \Omega^{-1}\sigma(t)\Omega$ and $\sigma(t)$ is arbitrary operator function. From the definition of $\Sigma(t)$ differential equation for Dyson's map $\Omega(t)$ may be seen

$$i\dot{\Omega} = \sigma(t)\Omega(t) \ . \tag{5.28}$$

From the knowledge of operators $\Omega(0)$ and $\dot{\Omega}(0)$ we obtain from equation (5.27) value of $\sigma(0)$. Solving the linear differential equation (5.26) than gives us explicit form of operator $\sigma(t)$. Finally, reconstruction of the Dyson's map $\Omega(t)$ is possible by means of equation (5.27).

We obtained a consistent time evolution picture including time dependent metric operator. The so called Coriolis term $\Sigma(t) = -i\Omega^{-1}\dot{\Omega}(t)$ occuring in the new generator $G(t)$ reflects the emergence of the manifest time-dependence of the inner products in the metric-endowed Hilbert space $\mathcal{H}^{(S)}$[66]. It is important to acknowledge that for time-dependent Dyson's map $\Omega(t)$ operator $G(t)$ doesn't satisfy the hidden Hermiticity condition (2.13). This means, that its spectrum may cease to be real and it cannot, in general, be interpreted as a quantum observable. It only serves as the generator of time-evolution.

5.3 Applications

The above outlined theory of time evolution in crypto-Hermitian quantum mechanics was in last years successfully applied to various issues like scattering [8], Ising quantum spin chain [24], Berry phase [26] or quantum control [66].

Also ambitious publications appeared in attempts to apply this formalism in quantum formulation of Big Bang [63, 65] or cannonical quantum gravity and quantum cosmology [39], where the two-component formulation of Wheeler-DeWitt equation is being used [37].

Example 4. We illustrate the formalism on the model of section 4.2 where we considered Hamiltonian K in the form of 2×2 real symmetric matrix.

The Schrödinger equation in $\mathcal{H}^{(F)}$

$$i\partial_t|\varphi(t)\rangle = \begin{pmatrix} 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 3 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} |\varphi(t)\rangle \tag{5.29}$$

is solved by evolution operator $U(t)$

$$U(t) = \begin{pmatrix} 0 & 0 & e^{-2it} & 0 \\ 0 & 0 & 0 & e^{-3it} \\ e^{-it} & 0 & 0 & 0 \\ 0 & e^{-it} & 0 & 0 \end{pmatrix}, \tag{5.30}$$

which satisfies the quasi-unitarity condition (5.10) and therefore guarantees the unitary time evolution in $\mathcal{H}^{(S)}$. Vectors in $\mathcal{H}^{(P)}$are evolved in time by unitary evolution operator

$$u(t) = \begin{pmatrix} e^{-i\frac{\gamma}{\alpha}t} & 0 & e^{-i\frac{\sqrt{2\alpha^2-\gamma^2}}{\alpha}t} & 0 \\ 0 & e^{-i\frac{\delta}{\beta}t} & 0 & e^{-i\frac{\sqrt{3\beta^2-\delta^2}}{\beta}t} \\ e^{-i\frac{\sqrt{2\alpha^2-\gamma^2}}{\alpha}t} & 0 & e^{i\frac{\gamma}{\alpha}t} & 0 \\ 0 & e^{-i\frac{\sqrt{3\beta^2-\delta^2}}{\beta}t} & 0 & e^{i\frac{\delta}{\beta}t} \end{pmatrix} . \tag{5.31}$$

Now, we admit manifest time dependence in the possible metric operators Θ. This means that our parameters α, β, γ, δ become functions of time $\alpha = \alpha(t)$, $\beta = \beta(t)$, $\gamma = \gamma(t)$ and $\delta = \delta(t)$. Hamiltonian H stays in its original time-independent form, but its Hermitian counterpart h may now become time-dependent $h = h(t)$

$$H = \Omega^{-1}(t)h(t)\Omega(t) . \tag{5.32}$$

Thus by allowing time dependency in the Dyson map, we can find broader class of similar Hermitian Hamiltonians for our original model H. Time-dependent Hermitian Hamiltonian h in $\mathcal{H}^{(P)}$is defined by

$$h(t) = \begin{pmatrix} \frac{\gamma(t)}{\alpha(t)} & 0 & \frac{\sqrt{2\alpha^2(t)-\gamma^2(t)}}{\alpha(t)} & 0 \\ 0 & \frac{\delta(t)}{\beta(t)} & 0 & \frac{\sqrt{3\beta^2(t)-\delta^2(t)}}{\beta(t)} \\ \frac{\sqrt{2\alpha^2(t)-\gamma^2(t)}}{\alpha(t)} & 0 & -\frac{\gamma(t)}{\alpha(t)} & 0 \\ 0 & \frac{\sqrt{3\beta^2(t)-\delta^2(t)}}{\beta(t)} & 0 & -\frac{\delta(t)}{\beta(t)} \end{pmatrix} . \tag{5.33}$$

We are also able to construct the generator $G(t) = H(t) + \Sigma(t)$ of time-evolution in $\mathcal{H}^{(S)}$

$$G(t) \begin{pmatrix} i\frac{\dot{\alpha}}{2} & 0 & -i\frac{\gamma}{\alpha}(1+\frac{A}{\alpha})\dot{\alpha} + 2i(1+\frac{\gamma B}{\alpha})\dot{\gamma} & 0 \\ 0 & i\frac{\dot{\beta}}{2} & 0 & -i\frac{3\delta}{2\beta}(1+\frac{C}{\beta})\dot{\beta} + 3i(1+\frac{\delta D}{\beta})\dot{\delta} \\ 1 & 0 & i(\frac{A}{2\alpha})\dot{\alpha} - iB\dot{\gamma} & 0 \\ 0 & 1 & 0 & i\frac{B}{2\beta}\dot{\beta} - iD\dot{\delta} \end{pmatrix} , \tag{5.34}$$

where

$$A = \frac{2\alpha^2+\gamma^2}{2\alpha^2-\gamma^2} , \quad B = \frac{\gamma}{2\alpha^2-\gamma^2} , \quad C = \frac{3\beta^2+\delta^2}{3\beta^2-\delta^2} , \quad D = \frac{\delta}{3\beta^2-\delta^2} . \tag{5.35}$$

Solution of the pair of Schrödinger equations (5.18), (5.19) would give us formulas for corresponding evolution operators $U_L(t)$ and $U_R(t)$.

Chapter 6

Perturbation approach

One of the necessary conditions of possible application of crypto-Hermitian quantum theory is reality of the spectrum. Schödinger form of Klein-Gordon equation (3.13) allows us to calculate the spectrum by means of analyzing the spectrum of operator

$$K = -\Delta + m^2 \ . \tag{6.1}$$

Until now we considered only the case of free Klein-Gordon equation, where the term m^2 equals to a constant. In this chapter we want to investigate behavior of Klein-Gordon equation with nonzero potential

$$K = -\Delta + V(\vec{x}) \ , \tag{6.2}$$

in particular we focus our attention to spherically symmetric Hamiltonians the spectrum of which would be analyzed be means of perturbation theory.

With the knowledge of spectrum of K, energy levels of Klein-Gordon equation are easily determined by the equation (3.24).

6.1 1/L perturbation method

The so called $1/L$ (or large-L) perturbation method, thoroughly described in [9],[11] or [18], allows us to compute bound states of spherically symmetric Hamiltonians. Schrödinger equation of such Hamiltonian can be rewritten in radial form

$$\left(-\frac{d^2}{dr^2} + \frac{L(L+1)}{r^2} + V(r)\right)\varphi(r) = \epsilon\varphi(r) \ , \tag{6.3}$$

where $L = (N-3)/2+l$ is positive integer, characterizing the angular momentum and N is the spacial dimension. The core of $1/L$ perturbation expansion technique lies in the fact, that in the regime of large L, the effective potential

$$V_{eff}(r) = \frac{L(L+1)}{r^2} + V(r) \tag{6.4}$$

reaches a pronounced minimum around which we can expand perturbation series.

$1/L$ perturbation method has been successfully applied not only on Hermitian models but on crypto-Hermitian models as well [19], [68], [6]. In what follows, we make use of this knowledge in connection with our non-Hermitian Klein-Gordon model.

6.2 Harmonic oscillator

First we try out the large-L perturbation method on a model of harmonic oscillator in spherical coordinates

$$\left(-\frac{d^2}{dr^2} + \frac{L(L+1)}{r^2} + \omega^2 r^2\right)\varphi(r) = \epsilon\varphi(r) \ . \tag{6.5}$$

It is an exactly solvable model with solutions [12]

$$\epsilon_{n,l} = 2\omega(2n + l + 3/2) \ . \tag{6.6}$$

By putting the first derivative equal to zero, we find the minimum of the effective potential (6.4)

$$V'_{eff} = -\frac{2L(L+1)}{r^3} + 2\omega^2 r = 0 \ . \tag{6.7}$$

We obtain binomial equation

$$r^4 = \frac{L(L+1)}{\omega^2} \ , \tag{6.8}$$

which has four different roots, $k \in \{1, 2, 3, 4\}$

$$R_k = e^{i\frac{k\pi}{2}} R \ , \quad R = \sqrt[4]{\frac{L(L+1)}{\omega^2}} \ . \tag{6.9}$$

Condition of the positiveness of the second derivative gives us the same integer for all four roots

$$V''_{eff} = \frac{6L(L+1)}{r^4} + 2\omega^2 = 8\omega^2 > 0 \ , \quad \forall k \ . \tag{6.10}$$

We choose the real positive root $k = 4$, $R_k = R$ and expand the potential function in Taylor series

$$V_{eff}(r) = 2\omega^2 R^2 + 4\omega^2 (r-R)^2 - \frac{4}{R}\omega^2 (r-R)^3 + \dots \ . \tag{6.11}$$

After substitution $r - R = \xi$ we obtain equation for eigenvalues

$$\left(-\frac{d^2}{d\xi^2} + 2\omega^2 R^2 + 4\omega^2 \xi^2 - \frac{4}{R}\omega^2 \xi^3 + \dots \right) \psi(\xi) = E\psi(\xi) \ . \tag{6.12}$$

In the lowest approximation of the large-L method, we can neglect all the terms of order R^{-1} and lower. Therefore we obtain well known energy spectrum of $1D$ harmonic oscillator

$$\epsilon_n = 2\omega^2 R^2 + 2\omega(2n+1) \ . \tag{6.13}$$

We can see that our approximative estimate corresponds with the exact spectrum (6.6) very well.

Now we can go back to the eigenvalues of the Klein-Gordon equation. According to (3.24), the relationship between just computed eigenvalues ϵ_n and eigenvalues E_n of Klein-Gordon equation is $E_n^{\pm} = \pm\sqrt{\epsilon_n}$. Hence for the energy levels of Klein-Gordon equation we have

$$E_n^{\pm} = \pm\sqrt{2\omega^2 R^2 + 2\omega(2n+1)} \ . \tag{6.14}$$

6.3 Anharmonic oscillator

We repeat the process from previous example on not exactly solvable model of quartic anharmonic oscillator

$$\left(-\frac{d^2}{dr^2} + \frac{L(L+1)}{r^2} + r^2 + \lambda r^4 \right) \varphi(r) = \epsilon\varphi(r) \tag{6.15}$$

From the first derivative of the effective potential we obtain sextic polynomial equation for the minimum

$$4\lambda r^6 + 2r^4 - 2L(L+1) = 0 \ . \tag{6.16}$$

Its real postive solution can be found as

$$R = \sqrt{\frac{A}{6\sqrt[3]{2}\lambda} + \frac{1}{3.2^{2/3}\lambda A} - \frac{1}{6\lambda}}\ , \tag{6.17}$$

where $A = \sqrt[3]{108\lambda^2 l^2 + \sqrt{(108\lambda^2 l^2 + 108\lambda^2 l)^2 - 4} + 108\lambda^2 l - 2}$.

Because $A > 0$ for $L = 1, 2, \ldots$ we can see that the second derivative is positive

$$V''_{eff}(R) = \frac{4A}{\sqrt[3]{2}\lambda} + \frac{8}{2^{2/3}\lambda A} + \frac{47}{6} > 0\ . \tag{6.18}$$

It means that we can expand Taylor series around the minimum

$$V_{eff}(r) = 2R^2+3\lambda R^4+(4+12\lambda R^2)(r-R)^2-4(R^{-1}+\lambda R)(r-R)^3+11(R^{-2}+2\lambda)+\ldots \tag{6.19}$$

Substitution $r - R = \xi R^{-1}$ leads us to the following eigenvalue problem

$$\left(-\frac{d^2}{d\xi^2} + 2R^2 + 3\lambda R^4 + 12\lambda\xi^2 + \ldots\right)\psi(\xi) = \epsilon\psi(\xi)\ , \tag{6.20}$$

which gives us in the first approximation energy spectrum of the harmonic oscillator

$$\epsilon_n = 2R^2 + 3\lambda R^4 + \sqrt{12\lambda}(2n+1)\ . \tag{6.21}$$

Now, we can investigate eigenvalues of the Hamiltonian $H = \begin{pmatrix} 0 & K \\ I & 0 \end{pmatrix}$

$$E_n^{\pm} = \pm\sqrt{2R^2 + 3\lambda R^4 + \sqrt{12\lambda}(2n+1)}\ , \tag{6.22}$$

which are real, thanks to positiveness of K.

Conclusion

In this thesis we searched for parallels and connections between relativistic and crypto-Hermitian quantum mechanics. We provided outline of relativistic wave equations, especially we reviewed thoroughly standard understanding and treatment of Klein-Gordon equation. We suggested different approach to the old issue of probability interpretation of Klein-Gordon equation. The crypto-Hermitian framework, into which it was set, was properly introduced and demonstrated on a few examples.

We managed to precisely apply all the outlined theory to a discretized model of Klein-Gordon operator. Including construction of the class of metric operators Θ and similar isospectral self-adjoint operators h. Subsequently, we enriched our theory with the investigation of the time-evolution of quantum system and the related problem of allowing manifest time-dependency in metric operator. We showed that the time-evolution of crypto-Hermitian operator with time-dependent metric is possible and satisfies the requirement on norm preservation of the evolving states. The formalism was illustrated on class of discrete models.

Innovative merge of crypto-Hermitian quantum theory and perturbation theory was applied on Klein-Gordon equation. In particular we chose the models of harmonic and anharmonic oscillator. Through the use of this approach we were able to reconstruct its eigenvalues with remarkable precision.

Crypto-Hermitian interpretation of Klein-Gordon equation is vital subject with broad unexplored areas. In this work we presented its further treatment mainly via discretization and perturbation theory.

In the future we see two main promising directions of deeper research. One going to proper interpretation of observed physical systems like pionic atom, including construction of exact metric operators. Second very ambitious vision goes to investigation of the rich parallels with quantum cosmology and possible applications in the quantum description of the Big Bang.

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Appendix

Appendix A

Riesz basis

Consider separable Hilbert space $\mathcal{H}$ with inner product $\langle\cdot|\cdot\rangle$ and basis $\{\zeta_n\}$. Is there an inner product $\langle\langle\cdot|\cdot\rangle$ on $\mathcal{H}$ with respect to which $\{\zeta_n\}$ is orthonormal?

For the finite-dimensional case the answer is always yes [42], there exists unique inner product that renders $\{\zeta_n\}$ orthonormal

$$\langle\langle\psi|\phi\rangle = \sum_{n=1}^{N} \overline{c_n} d_n \ , \tag{A.1}$$

where $\psi = \sum_{n=1}^{N} c_n \zeta_n$, $\phi = \sum_{n=1}^{N} d_n \zeta_n$ for some $\psi, \phi \in \mathcal{H}$.

Definition 6. A basis $\{\zeta_n\} \subset \mathcal{H}$ which is obtained from orthonormal basis $\{\xi_n\}$ through the action of an everywhere-defined bounded invertible linear operator $A : \mathcal{H} \mapsto \mathcal{H}$, i.e., $\zeta_n = A\xi_n$, is called a *Riesz basis*.

Definition 7. Inner product $\langle\cdot|\cdot\rangle_1$ is *topologically equivalent* to inner product $\langle\cdot|\cdot\rangle_2$ if and only if there exist positive real numbers c_1 and c_2 satisfying $c_1\langle\psi|\psi\rangle_2 \leq \langle\psi|\psi\rangle_1 \leq c_2\langle\psi|\psi\rangle_2$ for all $\psi \in \mathcal{H}$.

In the infinite-dimensional case such inner product may not exist. It holds that the inner product (A.1) that renders the basis $\{\zeta_n\}$ orthonormal and is topologically equivalent to $\langle\cdot|\cdot\rangle$ exists and is unique if and only if it is a Riesz basis [25].

Theorem 2. [42] H is crypto-self-adjoint, iff it has real spectrum and a Riesz basis of eigenvectors.

Appendix B

Complete biorthonormal system

Definition 8. Sequence $\{(\psi_n, \varphi_n)\}$ of ordered pairs of elements of H is called a *biorthonormal system* iff the following condition holds

$$\langle \psi_m | \varphi_n \rangle = \delta_{mn} \ . \tag{B.1}$$

Moreover, biorthonormal system is said to be *complete* if it satisfies

$$\sum_{n=1}^{N} |\psi_n\rangle\langle\varphi_n| = I \ . \tag{B.2}$$

It can be shown that every basis $\{\psi_n\}$ of separable Hilbert space $\mathcal{H}$ possesses a unique biorthonormal sequence $\{\varphi_n\}$ which is necessarily a basis itself [55].

Theorem 3 (Bari [25])**.** Let $\{\psi_n\}$ be the basis of $\mathcal{H}$. Than the biorthonormal system $\{(\psi_n, \varphi_n)\}$ exists and $\sum_{n=1}^{\infty} |\langle\psi_n|\psi\rangle|^2$ and $\sum_{n=1}^{\infty} |\langle\varphi_n|\psi\rangle|^2$ both converge for all $\psi \in \mathcal{H}$, if and only if $\{\psi_n\}$ is a Riesz basis.

In this case $\{\varphi_n\}$ is also Riesz basis. Than, in terms of biorthonormal system, each vector $\psi \in \mathcal{H}$ can be uniquely represented as

$$\psi = \sum_{n=1}^{\infty} \langle\psi|\varphi_n\rangle\psi_n \ . \tag{B.3}$$

The roles of $\{\psi_n\}$ and $\{\varphi_n\}$ are interchangeble, so it also holds that

$$\psi = \sum_{n=1}^{\infty} \langle\psi|\psi_n\rangle\varphi_n \ . \tag{B.4}$$

From theorem 2 we know that non-orthogonal eigenvectors $\{|\psi_n\rangle\}$ of crypto-Hermitian operator H form Riesz basis. Its associated biorthogonal basis is formed from eigenvectors $\{|\varphi_n\rangle\}$ of $H^\dagger$. The property of the biorthogonal system may be seen from relations

$$\lambda_m \langle \psi_m|\varphi_n\rangle = \langle H\psi_m|\varphi_n\rangle = \langle \psi_m|H^\dagger \varphi_n\rangle = \lambda_n \langle \psi_m|\varphi_n\rangle \ , \tag{B.5}$$

where λ_n are eigenvalues of both operators H and $H^\dagger$.

Spectral representation of crypto-Hermitian operator and its adjoint by means of the biorthonormal system

$$H = \sum_{n=1}^{N} \lambda_n |\psi_n\rangle\langle\varphi_n| \ , \quad H^\dagger = \sum_{n=1}^{N} \lambda_n |\varphi_n\rangle\langle\psi_n| \ . \tag{B.6}$$

Let $\{\psi_n\}$ be a Riesz basis creating biorthonormal system $\{(\psi_n, \varphi_n)\}$. We can construct unique inner product $\langle\langle\cdot|\cdot\rangle$ which makes $\{\psi_n\}$ orthonormal

$$\langle\langle\psi|\varphi\rangle = \sum_{n=1}^{N} \langle\psi|\varphi_n\rangle\langle\varphi_n|\varphi\rangle = \langle\psi|\Theta\varphi\rangle \ , \tag{B.7}$$

where we identified operator Θ with

$$\Theta\psi = \sum_{n=1}^{N} \langle\varphi_n|\psi\rangle\varphi_n \ . \tag{B.8}$$

Such defined operator Θ satisfies all the conditions on metric operator [42]. Thus, one of the possible ways how to construct metric operator for given crypto-Hermitian operator H is by use of the eigenvectors $|\varphi_n\rangle$ of its adjoint $H^\dagger$

$$\Theta = \sum_{n=1}^{N} \alpha_n |\varphi_n\rangle\langle\varphi_n| \ . \tag{B.9}$$

It has every-where defined inverse, defined analogically by its Riesz basis of eigenvectors.

$$\Theta^{-1} = \sum_{n=1}^{N} \alpha_n |\psi_n\rangle\langle\psi_n| \ . \tag{B.10}$$

The freedom in positive constants α_n arises from the fact emphasized in [59]. We can rescale our eigenvectors by means of arbitrary complex number κ_n

$$|\psi_n'\rangle = |\psi_n\rangle.\kappa_n \ , \quad |\varphi_n'\rangle = |\varphi_n\rangle.\frac{1}{\kappa_n} \tag{B.11}$$

and they still satisfy biorthonormality and completeness conditions. α is than given by $\alpha_n = \frac{1}{\kappa_n^* \kappa_n}$.