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Calculation of the metric in the Hilbert space of a $\mathcal{PT}$-symmetric model via the spectral theorem

David Krejčiřík

Department of Theoretical Physics, Nuclear Physics Institute, Academy of Sciences, 250 68 Řež near Prague, Czech Republic

E-mail: krejcirik@ujf.cas.cz

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Abstract

In a previous paper [1] we introduced a very simple $\mathcal{PT}$-symmetric non-Hermitian Hamiltonian with a real spectrum and derived a closed formula for the metric operator relating the problem to a Hermitian one. In this paper we propose an alternative formula for the metric operator, which we believe is more elegant and whose construction—based on a backward use of the spectral theorem for self-adjoint operators—provides new insights into the nature of the model.

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1. Introduction

Although quantum mechanics is conceptually a self-adjoint theory, there are a number of problems that require the analysis of non-self-adjoint operators. The study of resonances of self-adjoint Schrödinger operators via the technique of complex scaling [2] or the derivation of the famous Landau–Zener formula for the adiabatic transition probability between eigenstates of a time-dependent two-level system [3] are just two examples. However, in contrast to the well-understood theory of self-adjoint operators, the non-self-adjoint theory can be quite different (cf a nice review [4]) and is certainly less developed. The former is much easier to analyse because of the existence of the spectral theorem.

Recent years brought new motivations and focused attention to aspects of problems which attracted little attention earlier. A strong impetus comes from the so-called $\mathcal{PT}$-symmetric quantum mechanics, where the Hamiltonian H of a system is not Hermitian but the Schrödinger equation is invariant under a simultaneous change of spatial reflection $\mathcal{P}$ and time reversal $\mathcal{T}$ (cf [5] for the pioneering work and [6] for a recent review with many references). Here the interest consists of the fact that many of the $\mathcal{PT}$-symmetric Hamiltonians possess a real spectra and that the problem can be reinterpreted as an Hermitian one in a different Hilbert

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space. Indeed, and more generally, the identification is provided by the quasi-Hermiticity relation [7–10]:

$$H^*\Theta = \Theta H \tag{1}$$

valid on the domain of H. Here Θ is a bounded positive Hermitian operator, called metric.

There have been many attempts to calculate the metric operator Θ for the various $\mathcal{PT}$-symmetric models of interest (cf [1] for related references to which we add the Swanson model [11–13] and recent works [14, 15]). Most recent developments have come up with new efficient methods of how to calculate the metric [16–20], involving exact (non-perturbative) solutions in a compact form. Because of the complexity of the problem, however, it is not surprising that the majority of the available formulae for Θ are still approximative, usually expressed as leading terms of perturbation series.

Another problematic aspect of the available results is that the calculations are usually formal, partly because the boundedness of Θ is not always verified. However, the boundedness of the metric is a necessary condition, as addressed already in the original paper [7] and further emphasized in [21].

For these reasons we decided in [1] to introduce a new one-parametric non-Hermitian $\mathcal{PT}$-symmetric Hamiltonian H_α with a real spectrum and derived a formula for its metric Θ_α in a closed form and in a rigorous manner. These achievements were made possible by the manifest simplicity of our model: recalling the $\mathcal{PT}$-symmetric operators with general complex point interactions introduced by Albeverio, Fei and Kurasov in [22], our model can be roughly viewed as the Hamiltonian of a potential-free particle constrained to a bounded interval with two point-type interactions 'sitting' at the interval endpoints. In other words, we introduce a non-trivial coupling due to boundary conditions rather than to a local potential term. The calculation of the metric in [1] then relied on the fact that the eigenfunctions of H_α can be expressed explicitly in terms of trigonometric functions. Using the completeness of the latter, the metric operator was constructed by summing up certain trigonometric series.

The ultimate objective of this paper is to point out that the series determining Θ_α can be summed up alternatively—and probably more elegantly—by using the spectral theorem. Moreover, we believe that the resulting formula for the metric has a more transparent structure than that presented in [1]. Indeed, the individual terms of the present formula are well-known integral operators with explicit and extremely simple kernels (cf remark 4 below). We also hope that the simplicity of the formula will stimulate further study of the quasi-Hermiticity of our model, namely a (perturbative) computation of the square root of the metric operator and the corresponding Hermitian counterpart of H_α.

For the convenience of the reader we state here a simple version of the spectral theorem we shall use later:

Theorem 1 (Spectral theorem)**.** *Let H be a self-adjoint operator with compact resolvent in a Hilbert space with inner product $(\cdot,\cdot)$, antilinear in the first factor and linear in the second one. Then*

$$f(H) = \sum_{j=0}^{\infty} f(E_j)\psi_j(\psi_j,\cdot) \tag{2}$$

for any complex-valued, continuous function f. Here $\{E_j\}_{j=0}^{\infty}$ and $\{\psi_j\}_{j=0}^{\infty}$ denote respectively the set of eigenvalues and corresponding eigenfunctions of H.

We refer to [23, section VI.5] for a proof and a more general version of the spectral theorem when the compactness assumption is relaxed. Similar spectral decompositions hold also for normal operators, but they are in general false in the non-self-adjoint theory. Therefore it is remarkable that a modified version of (2) with $f(E) = E^n, n \in \mathbb{N}$, still holds for our non-Hermitian operator H_α (cf [1, proposition 4] for the case $n = 0$, the other cases being a consequence).

The spectral theorem is usually used to construct a function of a self-adjoint operator in terms of the sum of spectral projections. In this paper we use it backwards: we identify eigenprojections of a self-adjoint operator and replace an infinite series by a function of the operator. Unfortunately, the present method does not seem to be applicable in general. The reason why it works in the present model is that the eigenfunctions of H_α can be expressed in terms of eigenfunctions of self-adjoint operators.

In the forthcoming section 2 we recall the model introduced in [1] (we refer to that reference for more details and other results). This is followed by section 3 where the alternative formula for the metric is established.

2. The model

The underlying Hilbert space of the model introduced in [1] is the space of square-integrable functions $\mathcal{H} := L^2((0,d))$, where d is a positive number. While it is irrelevant that we consider an open interval in the definition of the Hilbert space, this choice turns out to be convenient when defining differential operators in $\mathcal{H}$ via the quadratic-form approach, since the corresponding Sobolev (energy) spaces are standardly defined over open sets only [24].

The simplicity of the Hamiltonian H_α defined in $\mathcal{H}$ is that it acts as the potential-free Hamiltonian

$$H_\alpha \psi := -\psi'' \quad \text{in} \quad (0,d),$$

while the non-Hermiticity enters uniquely through complex Robin boundary conditions

$$\psi'(0) + \mathrm{i}\alpha\psi(0) = 0 \qquad \text{and} \qquad \psi'(d) + \mathrm{i}\alpha\psi(d) = 0, \tag{3}$$

where α is a real constant. Using the quadratic-form approach, it was shown in [1] that H_α, with the domain $D(H_\alpha)$ consisting of all functions ψ in the Sobolev space $W^{2,2}((0,d))$ such that (3) holds, is an m-sectorial operator in $\mathcal{H}$. Note that the boundary terms in (3) are well defined because every element of $W^{2,2}((0,d))$ can be identified with a smooth function over $[0,d]$ in the sense of Sobolev embedding theorem [24]. The $\mathcal{PT}$-symmetry of our model is reflected by the relation

$$H_\alpha^* = H_{-\alpha},$$

where H_α^* denotes the adjoint of H_α.

Remark 1. A more general class of one-dimensional Schrödinger operators with non-Hermitian boundary conditions of the type (3) was studied previously by Kaiser, Neidhardt and Rehberg in [25]. In their paper—motivated by the needs of semiconductor physics, or more generally by regarding a quantum system as an open one—the parameter α is allowed to be complex but its imaginary part has opposite signs on the boundary points such that the system is dissipative. In our case (3), we actually deal with radiation/absorption boundary conditions in the language of theory of electromagnetic field.

It was also shown in [1] that the spectrum of H_α is purely discrete and given by

$$\sigma(H_\alpha) = \{\alpha^2\} \cup \left\{k_j^2\right\}_{j=1}^{\infty}, \qquad \text{where} \quad k_j := j\pi/d. \tag{4}$$

Moreover, all the eigenvalues are simple provided

$$\alpha d/\pi \notin \mathbb{Z}\setminus\{0\}. \tag{5}$$

Assuming this non-degeneracy condition, the eigenfunctions of the adjoint H_α^* corresponding to the eigenvalues counted as in (4) can be chosen as

$$\phi_j^\alpha(x) := \begin{cases} \chi_0^N + \rho_\alpha(x) & \text{if} \quad j = 0, \\ \chi_j^N(x) + \mathrm{i}\dfrac{\alpha}{k_j}\chi_j^D(x) & \text{if} \quad j \geqslant 1. \end{cases} \tag{6}$$

Here

$$\rho_\alpha(x) := \frac{\exp(\mathrm{i}\alpha x) - 1}{\sqrt{d}}$$

and $\{\chi_j^N\}_{j=0}^\infty$, respectively $\{\chi_j^D\}_{j=1}^\infty$, denotes the complete orthonormal family of the eigenfunctions of the Neumann Laplacian $-\Delta_N$, respectively Dirichlet Laplacian $-\Delta_D$, in $\mathcal{H}$

$$\chi_j^N(x) := \begin{cases} \sqrt{1/d} & \text{if} \quad j = 0, \\ \sqrt{2/d}\cos(k_j x) & \text{if} \quad j \geqslant 1, \end{cases} \qquad \chi_j^D(x) := \sqrt{2/d}\sin(k_j x).$$

Here the index for Dirichlet eigenfunctions runs over $j \geqslant 1$. Note that $-\Delta_N = H_0$ and that the spectrum of $-\Delta_D$ is equal to $\{k_j^2\}_{j=1}^\infty$.

3. Calculation of the metric

Still under the hypothesis (5), it was demonstrated in [1] that the operator

$$\Theta_\alpha := \sum_{j=0}^\infty \phi_j^\alpha(\phi_j^\alpha, \cdot) \equiv \operatorname*{s-lim}_{m\to\infty} \sum_{j=0}^m \phi_j^\alpha(\phi_j^\alpha, \cdot) \tag{7}$$

is bounded, symmetric, positive and satisfying (1) with H_α. Here $(\cdot, \cdot)$ denotes the inner product in $\mathcal{H}$, antilinear in the first factor and linear in the second one. Furthermore, a closed integral-type formula for the operator was derived by using known results about the sum of trigonometric functions.

Now we propose an alternative way how to sum up the infinite series in (7). First we write Θ_α as

$$\Theta_\alpha = P_0^\alpha + \Theta^{(0)} + \alpha\Theta^{(1)} + \alpha^2\Theta^{(2)}$$

with

$$\begin{aligned} P_0^\alpha &:= \phi_0^\alpha(\phi_0^\alpha, \cdot) = P_0^N + \chi_0^N(\rho_\alpha, \cdot) + \rho_\alpha(\chi_0^N, \cdot) + \rho_\alpha(\rho_\alpha, \cdot), \\ \Theta^{(0)} &:= \sum_{j=1}^\infty \chi_j^N(\chi_j^N, \cdot) = I - P_0^N, \\ \Theta^{(1)} &:= \sum_{j=1}^\infty \left(-\mathrm{i}k_j^{-1}\chi_j^N(\chi_j^D, \cdot) + \mathrm{i}k_j^{-1}\chi_j^D(\chi_j^N, \cdot)\right), \\ \Theta^{(2)} &:= \sum_{j=1}^\infty k_j^{-2}\chi_j^D(\chi_j^D, \cdot) = (-\Delta_D)^{-1}, \end{aligned}$$

where $P_0^N := \chi_0^N(\chi_0^N, \cdot) = P_0^0$ and I denotes the identity operator in $\mathcal{H}$. The equalities in the second and fourth lines follow directly by theorem 1 applied to $-\Delta_N$ and $-\Delta_D$, respectively. In order to use the spectral theorem in $\Theta^{(1)}$ as well, we introduce a 'momentum' operator p in $\mathcal{H}$ by

$$p\psi := -\mathrm{i}\psi', \qquad D(p) := W_0^{1,2}((0, d)). \tag{8}$$

The adjoint operator p^* acts in the same way but has a larger domain, $D(p^*) = W^{1,2}((0,d))$. Since χ_j^D and χ_j^N belong to $D(p)$ and $D(p^*)$, respectively, we have $p\chi_j^D = -\mathrm{i}k_j\chi_j^N$ and $p^*\chi_j^N = \mathrm{i}k_j\chi_j^D$. Consequently, theorem 1 yields

$$\Theta^{(1)} = p\sum_{j=1}^{\infty} k_j^{-2}\chi_n^D\left(\chi_n^D,\cdot\right) + p^*\sum_{j=1}^{\infty} k_j^{-2}\chi_n^N\left(\chi_n^N,\cdot\right)$$

$$= p(-\Delta_D)^{-1} + p^*\left(-\Delta_N^{\perp}\right)^{-1},$$

where $-\Delta_N^{\perp} := (I - P^N)(-\Delta_N)(I - P^N)$. Note that the 'interchange of summation and differentiation' in the first equality is justified just by the definition of the sum in (7) and the distributional derivative in (8).

Summing up, we get

Theorem 2. *The linear operator Θ_α in $\mathcal{H}$ defined by*

$$\Theta_\alpha = I + P_0^\alpha - P_0^N + \alpha p(-\Delta_D)^{-1} + \alpha p^*\left(-\Delta_N^{\perp}\right)^{-1} + \alpha^2(-\Delta_D)^{-1} \tag{9}$$

is bounded, symmetric, non-negative and satisfies (1) with H_α. Furthermore, Θ_α is positive if condition (5) holds true.

Note that the metric Θ_α tends to I as $\alpha \to 0$, which is expected due to the fact that H_0 coincides with the self-adjoint operator $-\Delta_N$.

Remark 2. Formula (9) can be written exclusively in terms of the operators p and p^* by employing the identities $-\Delta_D = p^*p$ and $-\Delta_N = pp^*$. Note also that the resolvent $(-\Delta_D)^{-1}$ and the reduced resolvent $\left(-\Delta_N^{\perp}\right)^{-1}$ are integral operators with explicit and extremely simple kernels (cf [23, example III.6.21].

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