PT-symmetric operators and metastable states of the 1D relativistic oscillators

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Abstract

We consider the one-dimensional Dirac equation for the harmonic oscillator and the associated second-order separated operators. Such operators, defined by complex dilation, give the resonances of the problem. Their unique extensions as closed operators with a purely point spectrum are PT-symmetric with positive eigenvalues converging to the Schrödinger ones as $\gamma \to \infty$. Precise numerical computations show that these eigenvalues coincide with the positions of the resonances up to the order of the width. The corresponding eigenfunctions are a definite choice of metastable states of the problem. Similar results are found for the Klein–Gordon oscillator: here also we have two closed, isospectral and complex conjugate extensions of the formal operator with PT-symmetry, but an infinite number of self-adjoint extensions and physical dynamics. The infinitely many pairs of eigenvectors of the two closed PT-symmetric operators give metastable states for any choice of the dynamics. The eigenvalues of the operator defined by complex dilation are resonances, although not according to the standard definition, for any dynamics.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

The harmonic oscillator is one of the fundamental dynamical systems both in classical and quantum theory [6] and the natural relativistic extensions have been investigated since a long time. In the relativistic quantum mechanics literature, therefore, one can find many different models that are considered relativistic oscillators [1–7]. These share the common property of reducing to the usual quantum oscillator in the Schrödinger limit but, otherwise, they present
large differences in the way the interaction is constructed. Obviously, different models have different dynamical and spectral properties: for instance, scalar potentials have been added to vector potentials in a phenomenological way with the purpose of stabilizing the system and giving confinement [8–11], or else the interaction has been obtained by adding to the free Dirac Hamiltonian a linear term in the position coordinate twisted by the Dirac $\beta$ matrix [12–18]. The relevance of such models in physics is clear and goes beyond their use for an elementary description of the confinement mechanism, in view of the connection with QFT and of the application of the Dirac equations to new materials [19], where the relativistic effects are more easily measured.

Here we call the spinor and scalar relativistic oscillator, respectively, the Dirac and the Klein–Gordon equations with a quadratic electrostatic potential because these models are very realistic and, in principle, can be experimentally implemented. Although they do not satisfy the necessary conditions for the exactness of the Foldy–Wouthuysen transformations [20, 21], it is obvious that the well-known harmonic oscillator is reproduced in the Schrödinger limit. Despite their apparent simplicity, however, the study of the relativistic electrostatic oscillators is not so easy as it looks at a first glance, but the results are satisfying.

Common wisdom tells us that strong instability is induced in quantum relativistic equations with unbounded potentials in the way described by the Klein paradox [22, 23]. Because of such instability the strongly bounded relativistic systems should present a continuous spectrum and complex resonances. This picture is well signified by a result that Plesset established in 1932 [24] and that can be summarized, with a rather paradoxical formulation, as follows: the Dirac equation with a minimal coupling that involves an electrostatic ‘bounding’ potential does not admit bound states. Of course, since bound states are present in the Schrödinger limit, the natural question that arises is what happens in the transition from a non-relativistic to a relativistic regime and in which sense this transition can be considered continuous in $1/c$. A first answer was given by Titchmarsh in [25] who studied in detail the perturbation treatment of the Dirac equation with piecewise linear vector potential. Due to the very cumbersome analytical calculations involved, the treatment was essentially restricted to the first perturbation order giving, however, some more explicit information on the properties of the continuous spectrum by investigating the Weyl function $m(\lambda)$ of the singular boundary value problem [26] in the complex plane. Very recently, numerical investigations of the Dirac equation with a linear and a quadratic electrostatic potential were presented in [27, 28], looking for a dissipative model: metastable states were found and the Schwinger pair production rate [29] was calculated in terms of the spectral concentration and in terms of the imaginary part of the resonances of the Dirac equation in external linear and quadratic potentials. In [27] the density of the states [30] was determined at finite values of $(1/c)$, finding a sum of Breit–Wigner lines whose width reproduced the pair production rate. In [28] the Dirac equation with a quadratic potential was revisited in the framework of the large-order perturbation theory. The singular problem gave rise to asymptotic non-oscillating series and the sum was calculated by the distributional Borel (DB) method, [31–35], coupled with a Padé approximation for the DB transform, finding complete agreement with [27]. Moreover, the spectral problem was clearly formulated stressing the reasons for the dissipative choice. It was also shown that this choice leads to the study of non-self-adjoint operators defined by complex dilation: the imaginary part of the complex energy levels, interpreted as resonances, again reproduces the pair production.

Although exact bound states do not exist, in this paper we show that particular metastable states can be identified. They are uniquely obtained from eigenvalues of the decoupled equations of Titchmarsh. At least for a small ratio of the interaction to the mass energy, they are well approximated. The role of the corresponding levels is similar to the role of the real part of the resonances. In this case we have both and it is our purpose to compare
them. Actually, for the metastable states, we have more exact results. In fact the Klein–Gordon-like Hamiltonians obtained by Titchmarsh in [25] (see also [36]) from the separation of the Dirac system of equations—hereby referred to as Titchmarsh operators—are uniquely defined closed operators with a discrete spectrum that gives the metastable states of the Dirac equation: we call metastable levels the energy values corresponding to the eigenvalues of the Titchmarsh operators. The Titchmarsh operators exhibit what in the current literature is known as the $PT$-symmetry, where $P$ is the parity transformation and $T$ the complex conjugation [1, 37, 38]: our paper, therefore, also adds a meaningful contribution to the discussion on the physical meaning of the $PT$-symmetric operators that still keep arising great interest (see, for instance, [39–43]). The metastable levels are studied in the next two sections. In section 2 we use the methods of the functional analysis supported by some recent results coming from the study of anharmonic quantum oscillators [37, 44] and give formal statements of our analytical results. We also show the possible role of the metastable levels as stationary levels of the separated $PT$-symmetric dynamics. In section 3 we then present the complex extensions of the position variables we have used, which have been introduced for two reasons: a better variational approximation and the connection with known results, mainly those of [37, 44]. In the final section, we present a discussion of the numerical results connecting the metastable levels to the resonances of the model. We thus have calculated some perfectly defined energy levels of the Titchmarsh operators stable at the Schrödinger limit and we have established their relationship to the real part of the resonances determined in [28] by the DB sum: we thus have proved that the difference is of the second order in the imaginary part of the resonances themselves and it can therefore be ascribed to the pair production rate, as it had to be expected on a physical ground. We have found that the best numerical way, reaching the very high precision necessary in order to compare the asymptotic behavior in a parameter $\Omega \sim O(1/\epsilon^2) \to 0$ with the DB sum of the power series expansion [28], is provided by a specialization of the Rayleigh–Ritz scheme [45] obtained through the matrix moment method [46, 47]. This method could also be used for higher values of $\Omega$ where, however, other approaches could be equally or even more efficient [27, 48].

2. The Dirac and the Klein–Gordon one-dimensional oscillators

Let us consider the one-dimensional Dirac equation in an electrostatic potential $V(x)$ [25, 36]. Using the notations of [25], we assume a two-component spinor wavefunction of the form $X = [X_1(x), X_2(x)]$ so that the explicit form of the Dirac equation reads

$$\frac{1}{c}(W + mc^2 - V(x))X_1(x) - \hbar \frac{d}{dx}X_2(x) = 0$$
$$\hbar \frac{d}{dx}X_1(x) - \frac{1}{c}(W - mc^2 - V(x))X_2(x) = 0.$$  (2.1)

We therefore see that the ‘large’ component of the spinor is $X_2(x)$. In the following, we will assume

$$V(x) = \frac{1}{2}m\omega^2x^2.$$  

We rescale the spatial coordinate as

$$x \mapsto \left(\frac{m\omega}{\hbar}\right)^{1/2}x,$$

so to make it dimensionless and we define the equally dimensionless parameters

$$\Omega = \left(\frac{\hbar\omega}{4mc^2}\right), \quad E = \frac{2}{\hbar\omega}(W - mc^2).$$
Here and in the following we will always take $\sqrt{\Omega} > 0$. Defining the formal Dirac Hamiltonian

$$\tilde{H}_D = \begin{pmatrix} x^2 - \frac{1}{\Omega} & \frac{1}{\sqrt{\Omega}} \frac{d}{dx} \\ -\frac{1}{\sqrt{\Omega}} \frac{d}{dx} & x^2 \end{pmatrix},$$

from (2.1) we then get the time-independent Dirac equation

$$\tilde{H}_D \Psi = E \Psi$$

and we recall that in [50–53] it was proved that any self-adjoint extension $H_D$ of $\tilde{H}_D$ has $\mathbb{R}$ as a continuous spectrum.

For our investigation we find it convenient to deduce separate second-order equations from the system (2.3), by introducing the linear combinations

$$\psi_+(x) = \frac{1}{\sqrt{2}} (X_1(x) + iX_2(x)), \quad \psi_-(x) = -i \frac{1}{\sqrt{2}} (X_1(x) - iX_2(x)),$$

which yield

$$\begin{align*}
\frac{d}{dx} \psi_+(x) - i \sqrt{\Omega} (E - x^2) \psi_+(x) &= \frac{i}{2 \sqrt{\Omega}} (\psi_+(x) + i \psi_-(x)) = 0 \\
\frac{d}{dx} \psi_-(x) + i \sqrt{\Omega} (E - x^2) \psi_-(x) + \frac{1}{2 \sqrt{\Omega}} (\psi_+(x) + i \psi_-(x)) &= 0.
\end{align*}$$

Solving the first equation in (2.5) in $\psi_-(x)$,

$$\psi_-(x) = -2 \sqrt{\Omega} \frac{d}{dx} \psi_+(x) + i (2E - x^2 + 1) \psi_+(x)$$

and substituting into the second equation, we finally find for $\psi_+(x)$ the second-order equation

$$\tilde{H}_+ (\Omega, E) \psi_+(x) = \lambda \psi_+(x),$$

where

$$\lambda = \lambda(\Omega, E) = E + \Omega E^2$$

and where the Titchmarsh operator

$$\tilde{H}_+ (\Omega, E) = -\frac{d^2}{dx^2} - 2i \sqrt{\Omega} x + (1 + 2E\Omega)x^2 - \Omega x^4$$

is a formal operator in the Hilbert space of the states $\mathcal{H} = L^2(\mathbb{R})$.

The assumption of a real energy $E$ will prove to be self-consistent with the boundary value problem in the sense that the formal PT-symmetric operator $\tilde{H}_+ (\Omega, E)$ extends uniquely to a closed and with purely point spectrum operator $H_+ = H_+ (\Omega, E)$, which also turns out to be PT-symmetric. The unstable term $-\Omega x^4$ is still present in $H_+$, suggesting that the Klein paradox arguments could be brought to bear: the imaginary term $-2i \sqrt{\Omega} x$ and the requirement of a purely point spectrum, however, make unique the extension $H_+$ which maintains the PT-symmetry of the formal operator $\tilde{H}_+$. Moreover, the unstable quartic term can be easily dealt with. Indeed in [37] a direct demonstration was given of the equality of the eigenvalues of a pair of quantum systems: the double well and the unstable anharmonic oscillator defined by complex translation, both of them, obviously, making sense and being well defined. In [44], then a general proof was presented that the spectrum of $H_+$ is discrete and positive:

$$\sigma(H_+) = \{ \lambda_n > 0 \}_{n \in \mathbb{N}}.$$ 

The unitarily equivalent adjoint Hamiltonian is
where $P$ is the parity transform and $T$ is the time reversal.

Note that the labeling of the levels is the same as we have at the Schrödinger limit, in the hypothesis that only one level is associated with one eigenvalue (see equation (2.12) below). We shall argue that this is the case and, moreover, we expect and prove the existence of infinitely many positive levels, stable at $\Omega = 0$. Let us now express our results in a formal way.

**Theorem 2.1.** For $E \in \mathbb{R}$ there is a uniquely defined closed extension with a purely point spectrum $H_+(\Omega, E)$ of the operator $\tilde{H}_+(\Omega, E)$. This extension is $\mathcal{PT}$-symmetric. The closed operator $H_-(\Omega, E)$ is then defined from (2.10).

**Proof.** We uniquely define the operator $H_+$ by the $L^2$ conditions at $\pm \infty$. The asymptotic behavior of the fundamental solution for $x \to +\infty$ is

$$
\Psi_+(x) \sim \frac{1}{x} \exp\left(i S(x) - \ln(x)\right) = \frac{1}{x} \exp\left(i S(x)\right),
$$

where

$$
S(x) = \int_0^x \sqrt{2} y^4 - (1 + 2E \Omega) y^2 \, dy \sim \sqrt{2} \frac{x^3}{3} \left(\frac{1 + 2E \Omega}{2\sqrt{2}}\right)x. \quad (2.11)
$$

The other independent solutions have the behavior

$$
\Phi_+(x) \sim \frac{1}{x} \exp\left(i S(x) + \ln(x)\right) = \exp\left(i S(x)\right).
$$

We have a similar problem at $-\infty$, with the fundamental solution

$$
\Psi_-(x) \sim \frac{1}{x} \exp(i S(x)) \quad \text{as} \quad x \to -\infty.
$$

The $\mathcal{PT}$-symmetry of the operator follows from the Green’s representation of the resolvent and the relation $\mathcal{PT}\Psi_+ = \Psi_-$. \hfill \Box

**Remark 2.1.** Let us stress that the spectrum of the operators $H_\pm$ is different from the spectrum of any self-adjoint extension of the Dirac matrix Hamiltonian (2.2): indeed, as previously observed, any such extensions have always $\mathbb{R}$ as a continuous spectrum, in agreement with the Klein paradox. This can be understood by observing that the coupling of the two equations (2.5) imposes a different domain in one (at least) of the operators $H_\pm$.

**Theorem 2.2.** Let $E \in \mathbb{R}$. The operator $H_-$ has an infinite number of positive simple eigenvalues $\lambda_n(\Omega, E)$, $n \in \mathbb{N}$. Correspondingly, there are infinitely many positive energy levels $E_n(\Omega)$ of the spectrum of $H_-$. The same happens for $H_+$.

**Proof.** Fix $\Omega, n \in \mathbb{N}$. In [44], the spectral problem $(L - \lambda) u(z) = 0$ was studied, with $L u(z) = -u''(z) - [a_0(iz)^m + P(iz)] u(z)$, $u(z)$ decaying to zero at infinity along the rays $\arg(z) = -\pi/2 \pm 2\pi/(m + 2)$ and $P(z) = a_1 z^{m-1} + \cdots + a_{m-1} z$, with $a_0 > 0$, $a_j \in \mathbb{R}$, $m \geq 2$. It was proved that if for some $1 \leq j \leq m/2$ it happens that $(j - k)a_k \geq 0$ for all $1 \leq k \leq m - 1$, then the eigenvalues are all positive and real. In our case with $m = 4$ and $a_0 = \Omega$, $a_1 = 0$, $a_2 = (1 + 2E \Omega)$, we have the result with the choice $j = 2$. Note that the operator $L$, as $H_-$, is defined by the subdominant behavior on the pair of sectors $S_{-1}, S_1$ (see remark 3.1 below). The proof equally applies to $H_+$ which is isospectral to $H_-$. Thus, from (2.7) and (2.8), we signify by ‘level’ any generalized eigenvalue $E_n > 0$, the solution of the implicit equation $\Omega E^2 + E = \lambda_n(E)$, which can be written as

$$
E = \frac{1}{2\Omega} \left(\sqrt{1 + 4\lambda_n(E) \Omega} - 1\right). \quad (2.12)
$$
The existence of a solution of (2.12) is proved in the following way. By real rescaling, and using the perturbation theory, we obtain, for fixed \( n, \Omega > 0 \) and large positive \( E \),

\[
\lambda_n(E) = \sqrt{1 + 2E\Omega(2n + 1 + \mathcal{O}(1/\Omega^3))} \ll E + \Omega E^2. \tag{2.13}
\]

The same behavior applies for \( E > 0 \) and small \( \Omega \), so that in this regime the solution of (2.12) is unique. \( \square \)

Let us now consider how these results can be brought to bear to the study of the Dirac equation. From (2.4) we see that the components \( X_1(x) \) and \( X_2(x) \) are linear combinations of two solutions \( \psi_+(x) \) and \( \psi_-(x) \) of the second-order equations. The eigenstates of the two Titchmarsh operators are independent because they are complex conjugate with non-vanishing real and imaginary parts, as can be seen from the equations and their asymptotic behaviors. If we take a pair of eigenfunctions \( (\psi_+(x), \psi_-(x)) \) of the separated equations such that \( \psi_+(x) = i\psi_-(x) \), this pair gives directly metastable states of the full problem, whereas the resonances give metastable states only by a cut-off: it is relevant that we have more exact information \([37, 44]\) on the metastable states than on the resonances. In the non-relativistic limit \( \Omega \to 0 \), the energy levels \( E_n(\Omega) \) tend to the eigenvalues \( E_n \) of the Schrödinger Hamiltonian and both the states tend to the real Schrödinger eigenstate \( \psi_n \) corresponding to \( E_n \). Recalling again (2.4) we also remark that, for the metastable states, \( X_2 \sim \text{Re} \psi_+ \) and \( X_1 \sim \text{Im} \psi_+ \). The sizes of the large and small components of the spinors, therefore, turn out to be different by many orders of magnitude, providing an approximation to the levels of the metastable states which is very natural and more accurate than the one we could obtain starting from the Schrödinger eigenvalues and perturbing them by means of the relativistic terms: indeed the metastable levels are approximated by the DBS that gives the sum of the complete perturbation series in \((1/c^2)\).

Take then the real operator

\[
\tilde{K}(\Omega, E) = \tilde{H}_c(\Omega, E) + 2i\sqrt{x} \tag{2.14}
\]

This is just the Klein–Gordon Hamiltonian with quadratic electrostatic potential and is defined as a closed \(\mathcal{PT}\)-symmetric operator \( K_+ \) by the behavior of the fundamental solutions,

\[
\Phi_\pm(x) \sim \frac{1}{|x|} \exp(iS(x)) \tag{2.15}
\]

as \( x \to \pm \infty \). \( K_+ \) has the positive eigenvalues \( \lambda_n \) for any real parameter \( E \) \([37, 44]\). Again the equivalent adjoint Hamiltonian,

\[
K_- = PK_+P = TK_+T = K_+^*,
\]

is obtained by parity transform. Following the same proof of theorem 2, we can show that there are \( \text{infinitely many positive energy levels} \) as in the Dirac case. The boundary conditions are similar to the resonance ones, but there are always \(\text{mixed conditions} \) Gamow, anti-Gamow at \( \pm \infty \). We define as the \(\mathcal{PT}\)-symmetric pair of dynamics the two non-unitary dynamics generated by the Hamiltonians \( K_\pm \). It is interesting to note that the energy levels are the same for the two dynamics, and that the two states are complex conjugate.

**Remark 2.2.** Let us stress that the small difference between \( H_c \) and \( \tilde{K} \) is, however, relevant: the formal operator \( \tilde{K} \) is in fact not uniquely implemented as a closed operator. In particular, we have infinite self-adjoint extensions with a discrete spectrum. Moreover, there is the closed extension defined by the Gamow condition at \( \pm \infty \), with eigenvalues considered resonances, in a generalized sense, given by the distributional Borel sum of the perturbation series.

In perfect analogy with the \( H_\pm \) operators, we consider a pair of isospectral \(\mathcal{PT}\)-symmetric operators \( K_\pm \) with positive simple eigenvalues. In this problem, where the physical dynamics...
does not exist because it is not unique, it is appropriate to consider as physical levels, in the first approximation, the values taken from the common eigenvalues of the pair of operators \( K_{\pm} \). The corresponding eigenstates of the pair of operators \( K_{\pm} \) and their combinations, as the real ones, are metastable states for all the infinite number of the unitary dynamics of the problem.

For the real energy \( E \), we have computed the eigenvalues of \( H_+ \) and \( K_+ \) by a variational method called the matrix moment method. Since each eigenvalue \( \lambda_n \) is positive \([44]\), we get the corresponding positive energy level \((2.12)\) holding both for the Dirac and the Klein–Gordon cases.

### 3. Definition of the Hamiltonians by subdominant behavior on two disjoint sectors

In this section we give the prescription for a non-ambiguous definition of the possible operators we can obtain from the formal operator \( \tilde{H}_+(\Omega, E) \) with positive parameters \((\sqrt{\Omega}, E)\). We follow the methods and the terminology of \([37, 59]\). Let us fix \( \text{arg}(ix) = \phi \), and consider the six sectors:

\[
S_j = \{ -\pi/6 < (\phi - j\pi/3) < \pi/6 \}, \quad -2 \leq j \leq 3.
\]

In particular, we define subdominant in the sector \( S_j \), \(-2 \leq j \leq 3\), the solution \( \psi_1j \) of the second-order equation, \( \tilde{H}(\Omega, E)\psi_j = 0 \), with the principal behavior for \( \phi = j\pi/3 \),

\[
\ln(\psi_1j(x)) = -\sqrt{\Omega} \frac{|x|^3}{3} (1 + O(|x|^{-2})) \quad \text{as} \quad |x| \to \infty. \tag{3.1}
\]

In certain cases, the \( L^2 \) behavior extends partially to the closure \( \tilde{S}_j \) of the angular sectors.

**Remark 3.1.** Observe that the \( PT \)-symmetric operators \( H_+ (\Omega, E) \) and \( K_+ (\Omega, E) \) are defined by the subdominant behavior on the pair of sectors \((S_{-2}, S_2)\) \([37, 44]\). Actually, the solutions respectively subdominant on the two sectors can be identified with the two fundamental solutions at \( \pm \infty \). In perfect analogy, the \( PT \)-symmetric operators \( H_- (\Omega, E) \) and \( K_- (\Omega, E) \) are defined by the subdominant behavior on the pair of sectors \((S_{-1}, S_1)\).

Let us now examine the complex contours that can be taken according to the operators we want to define.

(i) Complex translation and distortion. Let us start again from \( \tilde{H}_+ (\Omega, E) \) for positive \((\sqrt{\Omega}, E)\), as above. Consider next the complex translation

\[
\psi(x) \mapsto T_z \psi(x) = \psi(x + z),
\]

and the translated operator

\[
\tilde{H}^z = T_z \tilde{H}_+ T_{-z},
\]

\[
\tilde{H}^z(\Omega, E) = -\frac{d^2}{dx^2} - \Omega E^2 - E - 2i\sqrt{\Omega}(x + z) + (1 + 2E\Omega)(x + z)^2 - \Omega(x + z)^4. \tag{3.2}
\]

For \( z = iy, \ y > 0 \), \( \tilde{H}^z \) is uniquely defined as a closed operator \( H^z \) by the fundamental solutions

\[
\Psi^z_-(x) \sim \frac{1}{|x|^2} \exp(iS(x + z)), \tag{3.3}
\]

as \( x \to \pm \infty \), respectively. A relevant observation is in order. As the fundamental solutions are coincident with the subdominant solutions on the pair of sectors \((S_{-2}, S_2)\), we can prove that all the translated operators are isospectral with the operator defined by the subdominant condition on the two sectors above. Indeed it is easy to see that the fundamental solutions of
the translated operators are the translated of the fundamental solutions of $H_\nu(\Omega, E)$, with the behavior
\[
\Psi_{\pm}(x) \sim \frac{1}{|x|^2} \exp(iS(x)),
\]
as $x \to \pm \infty$, respectively. Since the eigenvalues are the zeros of the Wronskian of the two fundamental solutions, we can conclude that the translated operators are isospectral with the operator $H_\nu(\Omega, E)$ itself. In the numerical calculations, the translation parameter $y$ will be used as a variational parameter in the application of the Rayleigh–Ritz method. We could also consider the $PT$-symmetry conserving distortion of entire functions,
\[
\psi(x) \mapsto D\psi(x) = \sqrt{z'}(x)\psi(z(x)),
\]
where $z(x) = x(1 + it \tan(\pi/6)x \sqrt{1 + x^2})$ [60], yielding strictly sectorial operators,
\[
H^{\theta}_\nu(\Omega, E) = DH_\nu(\Omega, E)D^{-1}.
\]
These will be treated elsewhere.

\(\text{(ii) Complex dilation.}\)

Consider first the complex dilation
\[
\psi(x) \mapsto T_\theta \psi(x) = \psi(x \exp(i\theta)) = \psi^\theta(x),
\]
where $\psi(x)$ is restricted to the dense set of $L^2$ functions analytic on an angular sector
\[
\left| \frac{\text{Im} z}{\text{Re} z} \right| < \tan(\theta_0) \quad \text{with} \quad 0 < |\theta| < \theta_0 < \pi/6.
\]
The formal operators,
\[
\tilde{H}_\theta(\Omega, E) = T_\theta \tilde{H}_\nu(\Omega, E) T^{-1}_\theta,
\]
define the closed operators $H_\theta$ by the subdominant behavior on the two pairs of sectors $(S_{-2}, S_1)$ and $(S_{-1}, S_2)$ for negative and positive $\theta$, respectively, and are isospectral to the original operators with the same condition on the same sectors. For positive $\theta$ the fundamental solutions at $\pm \infty$ have the behavior
\[
\ln(\Psi^\theta_{\pm}(x)) = iS(x \exp(i\theta)) + O(\ln(|x|)),
\]
as $x \to \pm \infty$, respectively. For negative $\theta$ the fundamental solutions at $\pm \infty$ are
\[
\ln(\Psi^\theta_{\pm}(x)) = -iS(x \exp(i\theta)) + O(\ln(|x|)).
\]
We recall that in quantum mechanics the notion of resonance has its origin from the singularity of the scattering matrix [49] and is related to metastable states and spectral concentration [30].

In the framework of the Dirac theory, Titchmarsh considered the $|x|$ potential and found the resonances as the complex singularities of an analytic function [25], which, at the non-relativistic limit, become real and reproduce the eigenvalues of the Schrödinger equation. Later on, the method of analytic dilation for the computation of the resonances was introduced [54–56] and extended to the Stark effect in hydrogen [57, 58]: in this case the convergence of the DB sum of the perturbation series to the corresponding resonance was proved [35]. Here we apply this method to the two separated operators $\tilde{H}_\pm$, obtaining complex eigenvalues of the dilated operators $H^\theta_\pm$, coinciding for the two choices $\pm$, interpreted as resonances: indeed, the resonance operators $H^\theta_\pm$, defined by the subdominant behavior on the two pairs of sectors $(S_{-2}, S_1)$ and $(S_{-1}, S_2)$, have only eigenvalues. The two DB complex conjugate sums [31–35] apply to the energy levels of these operators defined by the subdominant behaviors on the two pairs of sectors $(S_{-2}, S_1)$ and $(S_{-1}, S_2)$, respectively: the standard request is the choice giving the negative imaginary part of the resonances. The application of the perturbation theory leading to the DB sums has been thoroughly studied in [28] by numerical methods, specializing, in particular, to the calculation of the pair production rate obtained from the imaginary part of the resonance.
4. Results

In order to compare the spectra of different boundary value problems, instead of integrating the differential equations as in [27], we have calculated the eigenvalues using a slight modification of the classical Weinstein–Aronszajn method [45] obtained from the theory of matrix moments [46], joint to the Newton procedure for finding the zeros of a function. In fact, due to the Jacobi form (4.1) of the Hamiltonian matrix in the base of the occupation number states, this is equivalent to a Rayleigh–Ritz variational scheme made more efficient through the matrix moments that shorten the computational time and increase the precision of the calculation.

We report in figure 1 the lowest energy levels of the metastable states, i.e. the first eigenvalues of the operators \( H_{\pm} \), of the Dirac 1D harmonic oscillator for different values of the parameter \( \Omega \).

We consider the translated \( H^{+}_{\pm} \), real \( K_{\pm} \) and dilated operators \( \tilde{H}_{\pm}(\theta) \) uniquely defined on \( L^{2}(\mathbb{R}) \). These are compressed on the space \( \mathcal{H}_{n} \) spanned by the first \( n \) Hermite eigenfunctions \( \{ \psi_{j} \}_{j \leq n} \) of the Schrödinger Hamiltonian \( H_{0} = p^{2} + \sigma^{2}x^{2} \), where \( \sigma \) is a variational parameter. The matrix elements \( H_{ik} \) of the fourth-degree polynomial in \( x \) are obviously dealt with by using the recurrence relation

\[
x h_{k} = (1/2) h_{k+1} + k h_{k-1}
\]

for the Hermite polynomials \( h_{k} \). The explicit relevant relations we are using read

\[
x^{2} h_{k} = (1/4) h_{k+2} + (k + 1/2) h_{k} + \sigma(k - 1) h_{k-2}
\]

\[
x^{3} h_{k} = (1/8) h_{k+3} + (3/4)(k + 1) h_{k+1} + (3/2) k^{2} h_{k-1} + k(k - 1)(k - 2) h_{k-3}
\]

\[
x^{4} h_{k} = (1/16) h_{k+4} + (1/4)(3 + 2k) h_{k+2} + (3/4)(2k^{2} + 2k + 1) h_{k} + k(2k - 1)(k - 1) h_{k-2}
\]

\[
+ k(k - 1)(k - 2)(k - 3) h_{k-4}.
\]

Thus, the general form of the matrix reads

\[
(H_{ik}) = \begin{pmatrix}
A_{0} & B_{0} & 0 & 0 & \cdots \\
C_{0} & A_{1} & B_{1} & 0 & \cdots \\
0 & C_{1} & A_{2} & B_{2} & 0 \\
\cdots & \cdots & \cdots & \cdots & \cdots
\end{pmatrix}
\]

(4.1)
Table 1. The lowest $d$-eigenvalue $E_{d0}$ for varying $\Omega$.

| $\Omega$     | $E_{d0}$                  |
|--------------|---------------------------|
| 0.0020       | 1.000 501 7620 + i 1.173 740 830 59 e-144 |
| 0.0025       | 1.000 627 7579 + i 9.420 791 109 45 e-116 |
| 0.0030       | 1.000 753 9782 + i 1.723 766 650 81 e-96  |
| 0.0035       | 1.000 880 4241 + i 9.775 439 246 61 e-83  |
| 0.0040       | 1.001 007 0969 + i 2.002 119 285 67 e-72  |
| 0.0045       | 1.001 133 9978 + i 2.081 656 038 53 e-64  |
| 0.0050       | 1.001 261 1278 + i 5.364 478 021 32 e-58  |

The first 4$\times$4 eigenvalues can be approximated by the eigenvalues of the Hamiltonian matrix truncated at the 4$\times$4th order. From the matrix moment theory [46], these eigenvalues are given by the zeros of the determinant of the matrix polynomials $P_n = P_n(\lambda)$, recursively defined in the following way:

\[
\begin{align*}
P_0 &= I_4 \\
P_1 &= B^{-1}_0(\lambda I_4 - A_0) \\
P_n &= B^{-1}_n(\lambda P_{n-1} - C_{n-2} P_{n-2} - A_{n-1} P_{n-1}),
\end{align*}
\]

$I_4$ being the 4 $\times$ 4 identity matrix. The solutions of $\det P_n(\lambda) = 0$ are indeed the 4$\times$4th-order Rayleigh–Ritz approximants that give upper bounds for the eigenvalues. Although lower bounds for the eigenvalues do not prove to be useful in our present context, it could however be observed that they can be obtained by this same method, looking for the zeros of the determinant of the matrix polynomial [47]

\[
P_n(\lambda) = P_n(0) P^{-1}_{n-1}(0) P_{n-1}(\lambda).
\]

Let us now present the numerical results. We denote by $', t, d'$ the quantities respectively related to the spectrum of the real, translated and dilated operators (2.14), (3.2) and (3.5) previously discussed. In table 1, for different values of $\Omega$, we give the complex $d$-eigenvalue $E_{d0}$ with lowest positive real part, reducing to the ground level in the non-relativistic limit. Since the effect to be highlighted is really tiny, these eigenvalues have been calculated with great accuracy, both in the arithmetic precision and in the number of iteration of the recurrence relation (4.2). The largest value of the latter has been taken to be 300: although a large number of decimal figures is already stabilized by few iterations, a very high precision is however necessary for a comparison of the $t$ with the $d$ eigenvalues, which we show here below. As expected, the results obtained in [27, 28] when studying the resonances of the Dirac equation by the spectral concentration and by the DB sum, as well as the asymptotic behavior of the imaginary part, are confirmed by the much more precise data given in table 1. In the application of the Rayleigh–Ritz method, we have used as variational parameters the size of the imaginary translation $y$ introduced in item (3.3) and the ‘frequency’ $\sigma$ of the operator $H_0$. 

where the symbols $A_n$, $B_n$ and $C_n$ represent $4 \times 4$ blocks given by

\[
\begin{align*}
(A_n)_{ik} &= H_{4n+i, 4n+k} \\
(B_n)_{ik} &= H_{4n+i, 4(n+1)+k} \\
(C_n)_{ik} &= H_{4(n+1)+i, 4n+k} = (B_n)_{ki}
\end{align*}
\]

with $n = 0, 1, 2, \ldots$ and $i, k = 0, 1, 2, 3$. 
There has been numerical evidence that the optimal values of these parameters are $1 \lesssim \gamma \lesssim 5$ and $1 \lesssim \sigma \lesssim 2$. In figure 2 we plot
\[ \Lambda = -\ln(E_{t0} - \text{Re}(E_{0})) \]
for a different number $n$ of iterations of (4.2) in order to test the stabilization of the data with $n$. We see that the saturation for decreasing values of $\Omega$ requires increasing values of $n$: it appears, however, that $n = 300$ is already sufficient for $\Omega = 0.0030$ and higher. The final value is almost coincident with minus twice the logarithm of the imaginary part of the eigenvalue $E_{t0}$, represented by the dashed horizontal lines.

**Remark 4.1.** This means that each eigenvalue of the operators $H_{\pm}$ is given by the distributional Borel sum of the perturbation series modulo a correction of the second order on the pair production effect (see [28]).

This property has been numerically checked by calculating the ratio $\Lambda/(-2 \ln(\text{Im}(E_{0})))$ for $0.0030 \leq \Omega \leq 0.0050$. A simple quartic Lagrangian interpolation on the data thus obtained gives 0.999 885 as a limiting value of the ratio.

We finally want to consider the influence of the imaginary term proportional to $\sqrt{\Omega}$ in (3.2). We have therefore calculated the difference of the first eigenvalue of the $(t)$ Dirac $PT$-symmetric operators $H_{\pm}$ and $(r)$ Klein–Gordon $PT$-symmetric operators $K_{\pm}$, respectively, and the ratio
\[ \kappa = (E_{t0}(\Omega) - E_{t0}(\Omega))/\Omega. \]
A least-squares computation on the data for $0.002 < \Omega < 0.005$ gives $\kappa = 0.9999539755 + 0.0284823904\Omega$, providing numerical evidence that the difference of the previous eigenvalues vanishes in the limit of a vanishing $\Omega$.

We have compared the differences of the second minus the first eigenvalue for the $t$ and $r$ operators:
\[ \delta = [(E_{t1}(\Omega) - E_{t0}(\Omega)) - (E_{r1}(\Omega) - E_{r0}(\Omega))]/\Omega, \]
finding a more than linear vanishing behavior with vanishing $\Omega$. 

**Figure 2.** The plot of $\Lambda = -\ln(E_{t0} - \text{Re}(E_{0}))$ versus the number $n$ of iterations of (4.2). Different symbols correspond to different values of $\Omega$. The horizontal dashed lines give $2 \ln(\text{Im}(E_{0}))$ for the corresponding $\Omega$. 

\[ n \]
\[ 150 \quad 200 \quad 250 \quad 300 \]
\[ 150 \quad 200 \quad 250 \quad 300 \]
\[ 0.0020 \quad 0.0025 \quad 0.0030 \quad 0.0035 \quad 0.0040 \quad 0.0045 \quad 0.0050 \]
\[ \Lambda \]
\[ 0.0020 \quad 0.0025 \quad 0.0030 \quad 0.0035 \quad 0.0040 \quad 0.0045 \quad 0.0050 \]
\[ n \]
5. Conclusions

In this paper we have completed the rigorous analysis of the basic model of the harmonic oscillator in the one-dimensional Dirac and Klein–Gordon theories, using recent mathematical results concerning the anharmonic oscillators and considering the relevance of the symmetries [37, 38]. As we said, the result is satisfying, since it leads one step closer to the QFT symmetries. In the Dirac case, we have shown that positive energy values, i.e. the metastable levels, can be obtained by the approximation of decoupling the Dirac system in two second-order equations and making the choice of a purely point spectrum, but without introducing a scalar potential, whose physical interpretation is usually uncertain. Although in the relativistic framework it is not possible or convenient to maintain all the principles of quantum mechanics, we can try to minimize the effects of the pair production by an approximate model. In fact in relativistic quantum mechanics, it is not required for a state to have a fixed number of particles and a unitary dynamics is therefore not necessary. We may still have, however, a $PT$-symmetric Dirac Hamiltonian with an infinite number of positive energy levels as in the non-relativistic case [37, 44]: the corresponding resonance operators are physically relevant but not so well known. Our numerical study shows that the positions of resonances and metastable levels are very close for a large value of $c$. We have also shown that the behavior of the Dirac equation appears very similar to that of the Klein–Gordon equation, where we have two $PT$-symmetric Hamiltonians and two complex conjugate sequences of metastable states, but a unique sequence of metastable levels [37, 44]. The investigation of the properties of the two- and three-dimensional relativistic oscillators will appear in a following paper.

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