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Solvability and $\mathcal{PT}$-symmetry in a double-well model with point interactions

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Abstract

The concept of point interactions offers one of the most suitable guides towards a quantitative analysis of properties of certain specific non-Hermitian (so-called $\mathcal{PT}$-symmetric) quantum-mechanical systems. This is illustrated with a double-well model, the easy solvability of which is shown to lead to a clear picture of the mechanisms of the unavoided level crossing and of the spontaneous $\mathcal{PT}$-symmetry breaking at a certain strong-non-Hermiticity boundary. Below this limit the model is shown to be suitable for an explicit illustration of technicalities related to the standard probabilistic physical interpretation of bound states in $\mathcal{PT}$-symmetric quantum mechanics.

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1. Introduction

A consistent probabilistic interpretation of bound states $|\psi\rangle$ in quantum mechanics requires that their norm is conserved in time [1]. In the light of the well-known Stone's theorem this means that their time-evolution must be unitary so that the generator of this evolution (= the physical Hamiltonian $H_{\rm p}$) cannot be, apparently, non-Hermitian. Still, the concept of a 'non-Hermitian Hamiltonian' $H_{\rm n} \neq H_{\rm n}^{\dagger}$ is in more or less current use in many mathematical considerations (e.g., in perturbative calculations [2] or in the schematic models of gravity [3] or supersymmetry [4]) as well as in various phenomenological studies (e.g., in nuclear physics [5], solid-state physics [6], particle physics and field theory [7] or in model building in magnetohydrodynamics [8] and cosmology [9]).

In such a context the use of solvable point interactions seems to offer a natural background for a simplification of some mathematical challenges [10] or of technical problems [11] as well as for an improvement of the feasibility of numerical calculations [12] and for a deepening of the related physical interpretation of the underlying dynamical processes

[13, 14]. In our paper we shall address several aspects of non-Hermiticity in this framework, especially those which were recently studied using the comparatively less easily tractable piecewise constant potentials [15]. We feel encouraged by the success and impact of these studies which have already found applications in supersymmetric quantum mechanics [16] and which seem to exhibit certain promising phenomenological (e.g., localization) properties [17].

We are persuaded that the class of point-interaction models could be even more capable of throwing new light on some of the paradoxes connected with the non-Hermiticity. We are going to pay attention to one of the most elementary representatives of this class which is just a simplified form of the potential which we already analysed in our older, purely numerical study [12] (cf also [13]). As long as all the similar models combine solvability (i.e., simplicity) with flexibility (controlled by several real parameters) we believe that there are good chances of an explicit confirmation of their full compatibility with the standard quantum theory. Here we are going to perform the first steps in this direction.

2. A zoo of non-Hermitian Hamiltonians

Our present study is motivated by the fact that in the light of our introductory comment the use of non-Hermitian Hamiltonians sounds like a paradox. Still, in the literature one may note an emergence of various sophisticated possibilities of making many of these models compatible with the concepts of physical observability [5, 18], with the standard principle of correspondence [19, 20] or with the introduction of relativistic kinematics [21], etc.

2.1. Quasi-Hermitian Hamiltonians

In a preliminary remark let us remind the reader that even many finite-dimensional non-Hermitian matrices $A \neq A^\dagger$ may be re-interpreted as Hermitian after one re-defines the scalar product of the two complex N-dimensional vectors $\vec{f}$ and $\vec{g}$ accordingly,

$$\left[(\vec{f},\vec{g})_{(I)} = \sum_{n=1}^{N} f_n^* g_n \equiv \langle f|g\rangle \right] \longrightarrow \left[(\vec{f},\vec{g})_{(\mu)} = \sum_{n=1}^{N} \left(\sum_{m=1}^{N} f_m^* \mu_{mn} \right) g_n \equiv \langle\langle f|g\rangle \right].$$

In the other words, one may simply abandon the most common definition of the bra vector $\langle f|$ (using the mere operations of transposition and complex conjugation) and replace it by its more general alternative with the symbol $\langle\langle f|$ dependent on the pre-selected metric $\mu = \mu^\dagger > 0$.

The same generalization will also work for Hilbert spaces with $N = \infty$ after a few necessary but entirely straightforward additional technical qualifications [5, 20]. One only has to keep in mind that any modification of the metric $I \to \mu$ specifies a different, μ-dependent Hermitian conjugation mapping $A \to A^\ddagger$,

$$A^\ddagger = (\mu A \mu^{-1})^\dagger, \qquad \mu = \mu^\dagger. \tag{1}$$

This means that the class of corresponding 'Hermitian' matrices $A = A^\ddagger$ varies with μ. In order to avoid confusion, let us call the matrices $A = A^\ddagger$ *quasi-Hermitian* (= the name introduced in [5]) whenever the positive definite metrics μ becomes different from the trivial identity operator I.

Any such specific metric operator $\mu > 0$ will be denoted by the symbol η in what follows. We must be careful with this convention since Dirac [22] used the same symbol η without requiring its positivity. This means that he spoke about a pseudo-metric μ, very well

exemplified by the indefinite Pauli matrix occurring in the paper by Feshbach and Villars [23] where $\mu = \sigma_3 \bigotimes I$. For this reason, the authors of [5] introduced another symbol for the metric ($\eta \to T$). Their choice proved unfortunate as it causes a highly undesirable confusion with the time-reversal symbol $\mathcal{T}$ so that recently, Mostafazadeh [17, 24] recommended the return to η with a specific subscript, $\eta \to \eta_+$. A less clumsy notation was preferred in [25] or [14] where one starts from a certain auxiliary parity-type indefinite operator $\mathcal{P}$ and then constructs the necessary alternative, 'physical' metrics as a positive-definite product $\eta \equiv \mathcal{QP}$ (where $\mathcal{Q}$ denotes the so-called quasiparity [26]) or $\eta \equiv \mathcal{CP}$ (with the operator of charge $\mathcal{C}$ [18]), respectively.

2.2. Non-quasi-Hermitian time-evolution generators

Beyond the 'mathematically safe' domain of quantum mechanics as covered by the majority of the current textbooks one may find a fairly broad 'grey zone' of models which do not seem to comply with all the postulates of the theory. One of the illustrations may be found in relativistic quantum mechanics [27] where several consequences of the time-evolution laws seem to be in conflict with the standard (e.g., probabilistic) postulates. For a brief explicit illustration of the possible difficulties encountered in similar cases, let us just recollect the exactly solvable Klein–Gordon model of [28],

$$(\mathrm{i}\partial_t)^2 \Psi^{(\mathrm{KG})}(x,t) = \hat{H}^{(\mathrm{KG})} \Psi^{(\mathrm{KG})}(x,t), \qquad H^{(\mathrm{KG})} = -\partial_x^2 + m^2(x)$$

where

$$m^2(x) = m_0^2 + \frac{B^2 - A^2 - A\omega}{\cosh^2 \omega x} + \frac{B(2A+\omega)\sinh \omega x}{\cosh^2 \omega x}. \tag{2}$$

Due to its exact solvability the model possesses the bound-state energies in closed form,

$$E_n^{(\pm)} = \pm\sqrt{m_0^2 - (A - n\omega)^2}, \qquad n = 0, 1, \ldots, n_{\max}, \qquad n_{\max} = \mathrm{entier}[A/\omega].$$

In the strong-coupling regime with $0 < m_0 < A$, a few low-lying states suffer a collapse and acquire, formally, complex energies, i.e., $\mathrm{Im}\big(E_0^{(\pm)}\big) \neq 0$, $\mathrm{Im}\big(E_1^{(\pm)}\big) \neq 0$ etc. We have certainly left the domain of quantum mechanics.

Once we stay within the interval $0 < A < m_0$, the strength of the force remains weak and we have well-behaved eigenvalues and bound states at all the admissible indices n. The time evolution of the system is generated by the 'non-Hermitian Hamiltonian' of [28]. We may abbreviate $\varphi_1^{(\mathrm{FV})}(x,t) = \mathrm{i}\partial_t \Psi^{(\mathrm{KG})}(x,t)$ and $\varphi_2^{(\mathrm{FV})}(x,t) = \Psi^{(\mathrm{KG})}(x,t)$ and arrive at the standard Schrödinger-like time-evolution equation

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

where the relativistic Feshbach–Villars-type Hamiltonian $\hat{h}^{(\mathrm{FV})}$ is not only manifestly non-Hermitian,

$$[\hat{h}^{(\mathrm{FV})}]^\dagger = \mathcal{P}\hat{h}^{(\mathrm{FV})}\mathcal{P}^{-1}, \qquad \mathcal{P} = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix},$$

but also non-quasi-Hermitian since $\det \mathcal{P} = -1$. As a 'candidate for the metric' the operator $\mathcal{P}$ is unacceptable because it is not positively definite.

In a way coined by Mostafazadeh [29], all the operators $A = A^\ddagger$ with an indefinite $\mu = \mathcal{P}$ may be called *$\mathcal{P}$-pseudo-Hermitian*, assuming only that the 'pseudo-metric' $\mathcal{P}$ in our Hilbert–Krein space [30] remains invertible. Keeping in mind the paramount importance of

the Klein–Gordon equation we probably should accept and tolerate the occurrence of similar time-evolution generators in physics. Recently, they became quite useful and popular in statistical physics [31] and also beyond the domain of quantum theory [32].

2.3. $\mathcal{PT}$-symmetric Hamiltonians

Our choice of the symbol $\mathcal{P}$ was equally strongly inspired by its role as a pseudo-metric *and* by its coincidence with the specific parity operator in Bender's and Boettcher's pioneering letter [33]. They paid attention to the bound states in complex potentials on a line,

$$V(x) \sim (\mathrm{i}x)^{2+\delta}, \qquad x \in \mathbb{R}, \qquad \delta \in (-1, 2) \tag{3}$$

which exhibit an unusual, antilinear parity and time-reversal symmetry,

$$\mathcal{PT}V(x) = V(x)\mathcal{PT} \tag{4}$$

where $\mathcal{P}$ is parity and the symbol $\mathcal{T}$ denotes the time-reflection operator [34]. Under condition (4) the real bound-state energies may be shown to emerge for an unexpectedly broad range of parameters [35].

Although symmetry (4) may be found in older literature (cf [36] and [37] working with $\delta = 2$ and $\delta = 1$, respectively), the importance of the letter [33] lies in the courage with which its authors opened the discussion of the possible sensibility of the study of non-quasi-Hermitian models in quantum mechanics. They had to meet a number of objections, a particularly concise sample of which was later formulated by R F Streater on his web page [38]. Fortunately, a key breakthrough occurred in several subsequent parallel studies of $\mathcal{PT}$-symmetric Hamiltonians, i.e., of the time-generators H such that $H\mathcal{PT} = \mathcal{PT}H$ or, equivalently, $H^\dagger = \mathcal{P}H\mathcal{P}$ whenever it is assumed that $\mathcal{P}^{-1} = \mathcal{P}$. In these studies people paid attention to the exactly solvable differential-equation models with forces (2) [39] or (3) [19] or to their linear-algebraic diagonal-matrix reformulations [40]. It has been clarified that the 'input' pseudo-Hermiticity of a given H may and must be complemented by another, positively definite (though, of course, H-dependent) metric η. Then, the pseudo-Hermitian Hamiltonians re-acquire the quasi-Hermiticity property

$$H^\dagger = \eta H \eta^{-1}, \qquad \eta = \eta^\dagger > 0. \tag{5}$$

All the requirements are being reduced to an *explicit* assignment of the *second*, 'physical' metric η to a given Hamiltonian H. One could speak about an 'exotic', $\mathcal{PT}$-symmetric version of standard quantum mechanics.

3. Point-interaction toy model

The vast majority of all the applications of $\mathcal{PT}$-symmetric quantum mechanics (PTSQM) will rely upon the assumption that for a given $\mathcal{P}$-pseudo-Hermitian quantum Hamiltonian H we find a physical metric operator η which is not too complicated. Most often, the consistent theory is expected to be based on the factorized form of the metric $\eta = \mathcal{CP}$ defined in terms of an involutive symmetry $\mathcal{C} = \mathcal{C}^{-1}$ (= 'charge' [14, 18, 41] or 'quasi-parity' [26, 39, 42]).

The sufficiently simple form of $\mathcal{C}$ or η may only be assigned to a sufficiently simple 'input' operator H. In this sense, all the $\mathcal{PT}$-symmetric models using point interactions [10, 12, 13] represent one of the most natural playgrounds for the explicit construction of η or $\mathcal{C}$. In such a context we reported [12] a few purely numerical results of the study of a one-dimensional Schrödinger equation

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)\right]\psi(x) = E\psi(x) \qquad \psi(\pm L) = 0 \tag{6}$$

with a double-well point-interaction $\mathcal{PT}$-symmetric potential $V(x)$ with complex couplings. In our present, non-numerically oriented continuation of this study let us first perform a trivial re-scaling of the interval of coordinates which replaces the usual large though fixed and finite cut-off parameter $L \gg 1$ by the more comfortable value $L = 1$. Secondly, let us slightly simplify the potential of [12] to a mere two-parametric $\mathcal{PT}$-symmetric double-well model

$$V(x) = -\mathrm{i}\xi\delta(x+a) + \mathrm{i}\xi\delta(x-a) \qquad x \in (-1,1) \tag{7}$$

where the potential is reduced to a mere pair of delta functions proportional to a purely imaginary coupling of size ξ and located at a distance measured by the variable $a \in (0,1)$.

3.1. Construction of the exact solutions

We have to solve equation (6) with the Dirichlet boundary conditions $\psi(\pm 1) = 0$ and with the piecewise-constant potential (7) equivalent to the two matching constraints

$$\frac{\mathrm{d}}{\mathrm{d}x}\psi(\pm a + 0) - \frac{\mathrm{d}}{\mathrm{d}x}\psi(\pm a - 0) = \pm\mathrm{i}\xi\psi(\pm a). \tag{8}$$

This task will be facilitated by the observation (based on the inspection of equation (8) at small ξ) that our potential (7) represents a smooth perturbation added to the solvable (and safely Hermitian) bound-state problem in an infinite square well which possesses a well known and safely real discrete and positive spectrum. This means that the proof of the reality and positivity of the energies E_n remains trivial in the weak-coupling regime. We may assume that $\xi \in (0, \xi_{\mathrm{crit}})$, being aware that the quantity ξ_{crit} may vary with both the shift a and excitation n. This makes the explicit estimates of the maximal allowed coupling ξ_{crit} important. Their determination will be discussed later. Now, we only put $E = \kappa^2$ and recollect the usual PTSQM normalization convention

$$\psi(x) = \psi_S(x) + \mathrm{i}\psi_A(x), \qquad \psi_S(x) = \psi_S^*(x) = \psi_S(-x), \qquad \psi_A(x) = \psi_A^*(x) = -\psi_A(-x)$$

which significantly facilitates an ansatz for the wavefunctions,

$$\psi(x) = \begin{cases} \psi_L(x) = (\alpha - \mathrm{i}\beta)\sin\kappa(x+1), & x \in (-1,-a) \\ \psi_C(x) = \gamma\cos\kappa x + \mathrm{i}\delta\sin\kappa x, & x \in (-a,a) \\ \psi_R(x) = (\alpha + \mathrm{i}\beta)\sin\kappa(-x+1), & x \in (a,1). \end{cases} \tag{9}$$

Together with the formula for their derivatives,

$$\psi'(x) = \begin{cases} \psi_L'(x) = \kappa(\alpha - \mathrm{i}\beta)\cos\kappa(x+1), & x \in (-1,-a) \\ \psi_C'(x) = -\kappa\gamma\sin\kappa x + \mathrm{i}\kappa\delta\cos\kappa x, & x \in (-a,a) \\ \psi_R'(x) = -\kappa(\alpha + \mathrm{i}\beta)\cos\kappa(-x+1), & x \in (a,1) \end{cases} \tag{10}$$

both these formulae enter the matching constraint (8) and transform it into the following four-by-four matrix equation,

$$\begin{pmatrix} \sin\kappa(1-a) & 0 & -\cos\kappa a & 0 \\ 0 & \sin\kappa(1-a) & 0 & -\sin\kappa a \\ -\cos\kappa(1-a) & \xi\kappa^{-1}\sin\kappa(1-a) & \sin\kappa a & 0 \\ \xi\kappa^{-1}\sin\kappa(1-a) & \cos\kappa(1-a) & 0 & \cos\kappa a \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \\ \gamma \\ \delta \end{pmatrix} = 0. \tag{11}$$

It possesses nontrivial solutions if and only if its secular determinant $\mathcal{D}(\kappa)$ vanishes,

$$\mathcal{D}(\kappa) \equiv -\frac{1}{2}\left\{\sin 2\kappa + \frac{\xi^2}{\kappa^2}\sin 2\kappa a \sin^2[\kappa(1-a)]\right\} = 0. \tag{12}$$

The sequence of nodal zeros $\kappa_n = \kappa_n(a,\xi) > 0$ of this trigonometric function determines the spectrum of the energies $E_n = \kappa_n^2 > 0$. The coefficients α, β, γ and δ define the wavefunction and are also given by the nice and compact formulae, say,

$$\gamma = \frac{\xi \sin\kappa a \sin\kappa(1-a)}{\kappa\cos\kappa}\delta, \qquad \beta = \frac{\sin\kappa a}{\sin\kappa(1-a)}\delta \tag{13}$$

$$\delta = -\frac{\xi \cos\kappa a \sin\kappa(1-a)}{\kappa\sin\kappa}\gamma, \qquad \alpha = \frac{\cos\kappa a}{\sin\kappa(1-a)}\gamma \tag{14}$$

with an appropriate choice of a convenient normalization.

3.2. Onset $\xi_{\rm crit}$ of the spontaneous $\mathcal{PT}$-symmetry breakdown

The compact solvability of our matching conditions enables us to determine the range of couplings ξ for which all the roots $\kappa_n = \kappa_n(a,\xi)$ of our secular equation (12) remain real. We shall see that it happens within fairly large intervals of $\xi \in [0, \xi_{\rm crit}(a)]$, at the upper end of which one encounters the generic merger and subsequent complexification of some of the low-lying energy pairs [30].

3.2.1. The reality of the energies in the weak-coupling regime. In the PTSQM context it is usually emphasized that after the transition through the point $\xi_{\rm crit}(a)$ (which is usually called an 'exceptional point' [43]), the complexification of the energies is accompanied by the (so-called spontaneous) breakdown of the $\mathcal{PT}$-symmetry of the wavefunctions. The rigorous study of this phenomenon proves significantly facilitated in our specific, solvable point-interaction model. Firstly we may drop the obvious zero root $\kappa = 0$ of equation (12) as spurious, giving just the trivially vanishing wavefunctions. Secondly, we may start our considerations from the domain of the very small $\xi \ll 1$ where it is easy to observe that the well-known square-well roots are only slightly perturbed during the growth of ξ,

$$\kappa_n(a,\xi) \approx \frac{n}{2}\pi + \mathcal{O}(\xi^2), \qquad n = 1, 2, \ldots. \tag{15}$$

With the further growth of ξ we note that the second term in equation (12) will be most influential at the smallest energy levels κ_n^2. The main uncertainty in an estimate of its effect lies in the a dependence of its trigonometric factor.

3.2.2. An explicit formula for $\xi_{\rm crit}(1/2)$. The mechanism of the spontaneous breakdown of the $\mathcal{PT}$-symmetry will be best visible in the most symmetric case with the half-unit displacement $a = 1/2$ of our δ-functional interaction points in equation (7). In the secular equation

$$\sin\kappa\left[\cos\kappa + \frac{\xi^2}{4\kappa^2}(1-\cos\kappa)\right] = 0, \qquad a = \frac{1}{2} \tag{16}$$

the odd-parity square-well roots (= those with even subscripts n in the zero-order equation (15)) will not move with the growth of ξ at all, due to the ξ independence of the first factor in equation (16). In contrast, the ξ dependence of the odd-n series of the roots will be nontrivial and controlled by their implicit definition (16) or, after a simplification, by the equation

$$\cos\kappa = -\frac{\mu^2}{\kappa^2 - \mu^2}, \qquad \mu = \frac{\xi}{2}. \tag{17}$$

Such a picture is extremely transparent because the right-hand-side curve is a smooth and growing function of $\kappa \geqslant 0$ with a single pole at $\kappa = \mu$. Its values are larger than one at the

smallest $\kappa \leqslant \mu$ where it cannot produce any roots since we must have $|\cos\kappa| \leqslant 1$. At all the larger $\kappa > \mu = \xi/2$ the latter curve is negative. Of course, it should not lie below the minus-one lower limit so that we may set an improved estimate of the roots as $\kappa > \sqrt{2}\mu = \xi/\sqrt{2}$. This is a constraint imposed, in effect, not only upon the energies κ^2 in a given potential but also upon the allowed measure ξ of the manifest non-Hermiticity at a given energy.

An inspection of equation (17) reveals that the growth of ξ implies that the first two ξ-dependent energy levels $E_1 = \kappa_1^2(1/2, \xi)$ and $E_3 = \kappa_3^2(1/2, \xi)$ move towards each other until they coincide at a certain critical strength $\xi_{\rm crit} = 2\mu_0$. We have $\kappa_1(1/2, \xi_{\rm crit}) = \kappa_3(1/2, \xi_{\rm crit}) = \nu_0 > \pi$ at this point. In other words, the left- and right-hand-side curves in equation (17) will touch at a point which is determined by the two coupled equations

$$\cos\nu_0 = -\frac{\mu_0^2}{\nu_0^2 - \mu_0^2}, \qquad -\sin\nu_0 = \frac{2\mu_0^2\nu_0}{\left(\nu_0^2 - \mu_0^2\right)^2}. \tag{18}$$

We eliminate

$$\mu_0^2 = -2\nu_0\frac{\cos^2\nu_0}{\sin\nu_0}$$

and get the reduced equation for the remaining unknown,

$$\nu_0 = 2\tan\tfrac{1}{2}\nu_0\cos\nu_0.$$

We may find its root $\nu_0 \approx 3.874\,366\,817$ numerically, at $\mu_0 \approx 2.529\,882\,472$, i.e., at the critical strength $\xi_{\rm crit} \approx 5.059\,764\,944$.

The touching-point $\xi_{\rm crit}$ will grow with the excitation. We may conclude that the spectrum remains real at *all* the couplings $\xi \leqslant \xi_{\rm crit} \approx 5.06$. This means that the $\mathcal{PT}$-symmetry becomes spontaneously broken and some of the energies complexify *only* beyond this critical strength of the non-Hermiticity.

3.3. Unavoided crossings of the energy levels

3.3.1. Facilitated construction at $a = 1/2$. The touching point of the negative branch of the cosine with an increasing right-hand-side hyperbolic curve of equation (17) is displaced to the right of the first excited level, $\nu_0 > \kappa_2(1/2, \xi) = \pi$. The latter level was generated by the sine part of secular equation (16) and coincides with the position of the minimum of the cosine curve. We may conclude that as long as we had the ground-state level $\kappa_1(1/2, 0) = \pi/2$ at $\xi = 0$, the continuous and growing function $\kappa_1(1/2, \xi)$ of ξ crosses the line of $\kappa_2(1/2, \xi)$ at some particular coupling strength $\xi_{1\otimes 2}$ which lies somewhere inside the interval $(0, \xi_{\rm crit})$.

The existence of similar points of an unavoided crossing of the real energy levels has been spotted in several other solvable models [26, 44, 45]. In the present $a = 1/2$ illustrative example these unavoided crossings will involve all the pairs of the real levels $\kappa_{4m-3}(1/2, \xi)$ and $\kappa_{4m-2}(1/2, \xi)$. Their crossings are unique and will take place at the special strengths $\xi = \xi_{(4m-3)\otimes(4m-2)}$ defined by equation (16) which leads to the elementary formula

$$\xi_{(4m-3)\otimes(4m-2)} = \sqrt{2}\pi(2m-1), \qquad m = 1, 2, \ldots. \tag{19}$$

At these crossing points, our non-Hermitian Hamiltonian ceases to be diagonalizable and remains only block-diagonalizable, containing the so-called Jordan canonical irreducible triangular submatrices [46]. Whenever we wish to avoid similar subtleties, it suffices to assume that $\xi < \min(\xi_{(4m-3)\otimes(4m-2)}) = \xi_{1\otimes 2} = \sqrt{2}\pi \approx 4.442\,882\,938$.

3.3.2. Approximate constructions in the vicinity of $a = 1/2$. The remarkable factorization (16) of our general secular equation hints that in a small vicinity of $a = 1/2$ one could still expect simplifications. Introducing a small measure of perturbation σ let us write $a = 1/2 + \sigma/(2\kappa)$ and return once more to our exact secular equation (12) which reads, in the new notation,

$$\sin 2\kappa + \frac{\xi^2}{2\kappa^2}\sin(\kappa+\sigma)[1-(\kappa-\sigma)] = 0.$$

In the first two orders of σ the second term has the form of the product

$$\frac{\xi^2}{2\kappa^2}\left(\sin\kappa + \sigma\cos\kappa - \frac{1}{2}\sigma^2\sin\kappa\right)\left(1-\cos\kappa-\sigma\sin\kappa+\frac{1}{2}\sigma^2\cos\kappa\right)$$

so that we may study the following approximation of the secular equation:

$$\sin 2\kappa + \frac{\xi^2}{2\kappa^2}\left[\sin\kappa\,(1-\cos\kappa) - \sigma\,(1-\cos\kappa) - \frac{1}{2}\sigma^2\sin\kappa\right] = \mathcal{O}(\sigma^3). \tag{20}$$

First thing we note is that at $\sigma \neq 0$ the factorizability of equation (16) is lost so that one cannot factor the term $\sin\kappa$ out. This means that all the sine-generated roots $\kappa_2(a,\xi)$, $\kappa_4(a,\xi)$, $\kappa_6(a,\xi)$, ... (which were ξ independent at $\sigma = 0$) may become ξ dependent even near the square-well regime with very small $\xi \approx 0$.

Within our precision of $1 + \mathcal{O}(\sigma^3)$ let us employ the partially factorized approximate secular equation (20),

$$\sin\frac{1}{2}\kappa\left\{4\cos\frac{1}{2}\kappa\cos\kappa + \frac{\xi^2}{2\kappa^2}\left[2\sin\kappa\sin\frac{1}{2}\kappa - 2\sigma\sin\frac{1}{2}\kappa - \sigma^2\cos\frac{1}{2}\kappa\right]\right\} = 0.$$

In its light the subset of the roots $\kappa_4(a,\xi)$, $\kappa_8(a,\xi)$, $\kappa_{12}(a,\xi)$, ... still remains more or less ξ independent at the sufficiently small $\sigma \sim a - 1/2$. For the complementary family with the safely non-vanishing $\sin\frac{1}{2}\kappa$ we get, in the first nontrivial approximation, the implicit definition

$$\cot\frac{1}{2}\kappa\cos\kappa + \frac{\xi^2}{4\kappa^2}[\sin\kappa - \sigma] = 0$$

which indicates that all the roots $\kappa_2(a,\xi)$, $\kappa_6(a,\xi)$, $\kappa_{10}(a,\xi)$, ... which annihilated $\cos(\kappa/2)$ at $\alpha = 1/2$ (i.e., at $\sigma = 0$) will now grow with σ. As one can easily demonstrate, they will all move in proportion to the factor $\xi^2/4\kappa^2$ at small ξ.

We may conclude that although the study of our toy model in the domain where $a - 1/2$ does not vanish is perceivably more complicated in the technical sense, a straightforward perturbative approach to a systematic derivation of the $\mathcal{O}(\sigma^k)$ corrections is still feasible. Hence, we may recommend it as a complement or alternative to the less sophisticated numerical constructions.

Skipping the details we shall now return to $a = 1/2$ and show how our model may be interpreted as a mere small perturbation of its Hermitian square-well $\xi \to 0$ limit.

4. The excitation dependence of the solutions

Our construction of the solutions need not necessarily be only based on the purely numerical determination of the roots κ_n from transcendental equations. Alternatively, perturbative methods are also easy to apply, especially when $\kappa_n = \mathcal{O}(n)$ is large.

4.1. A power-series analytic representation of the energies

Whenever the value of ξ stays safely below the $\mathcal{PT}$-symmetry breakdown boundary $\xi_{\rm crit} \approx 5$, all the roots $\kappa_n(a,\xi)$ of our secular equation (12) with $n = 1, 2, \ldots$ converge to their compact square-well limits $\kappa_n(a,0) = n\pi/2$ not only when we move $\xi \to 0$ but also for the growing $n \to \infty$. In order to describe this phenomenon in more detail, let us return to the secular equation (16) where we may skip the trivial case (= even-subscripted closed solutions $\kappa_{2m}(1/2,\xi) \equiv m\pi$ with $m = 1, 2, \ldots$) and introduce the following new variables for the odd-subscripted roots,

$$\kappa_{4m-3} = \frac{(4m-3)\pi}{2} + x_m, \qquad \kappa_{4m-1} = \frac{(4m-1)\pi}{2} - y_m, \qquad m = 1, 2, \ldots . \tag{21}$$

This simplifies the secular sub-equation (17) which forms the series of equations

$$\sin x = \frac{1}{L^2(m,x) - 1}, \qquad L(m,x) = \frac{(4m-3)\pi + 2x}{2\mu}, \qquad m = 1, 2, \ldots, \tag{22}$$

for the unknown $x = x_m$ and another, slightly different series for $y = y_m$,

$$\sin y = \frac{1}{U^2(m,y) - 1}, \qquad U(m,y) = \frac{(4m-1)\pi - 2y}{2\mu}, \qquad m = 1, 2, \ldots . \tag{23}$$

The roots remain bounded, $x_n < \pi$ and $y_m < \pi$, but they depend on both the coupling $\mu = \xi/2$ and index m. As long as equations (22) and (23) are not too dissimilar, we may treat them as two special cases of a single equation,

$$\sin z = \left[\left(\frac{1}{\lambda\mu} - \frac{z}{\mu} \right)^2 - 1 \right]^{-1}, \qquad z = \begin{cases} x_m \\ y_m \end{cases}, \qquad \lambda = \begin{cases} -\dfrac{2}{(4m-3)\pi} \\ +\dfrac{2}{(4m-1)\pi}. \end{cases} \tag{24}$$

Once λ is small, it is trivial to solve it in closed form, say, by iterations,

$$z = \lambda^2\mu^2 + \lambda^4\mu^4 + 2\lambda^5\mu^4 + \frac{7}{6}\lambda^6\mu^6 + 6\lambda^7\mu^6 + \left(7 + \frac{3\mu^2}{2} \right) \lambda^8\mu^6 + \mathcal{R}(\lambda,\mu). \tag{25}$$

Here, the $\mathcal{O}\left(\lambda^9\mu^8\right)$ remainder has transparent structure

$$\mathcal{R}(\lambda,\mu) = \frac{40}{3}\lambda^9\mu^8 + \left(36 + \frac{83\mu^2}{40} \right) \lambda^{10}\mu^8 + \left(30 + \frac{80\mu^2}{3} \right) \lambda^{11}\mu^8 + \mathcal{O}(\lambda^{13}\mu^{10})$$

and admits further higher order improvements if needed. Note that this series is not changing signs which means that the function itself is monotonic and growing with $\lambda > 0$. It behaves like a perturbation series in both λ (inversely proportional to the excitation number m) and $\mu = \xi/2$ (the coupling) *simultaneously*.

4.1.1. A check of consistency. We may compare the rate of growth of x_m and y_m with an increase of the coupling μ. This requires a removal of the difference in the m dependence of the respective λ, via an obvious transition to the same, shared m-dependent factor τ,

$$z = \begin{cases} x_m \\ y_m \end{cases} \quad \Longrightarrow \quad \pi\lambda = \begin{cases} -\dfrac{2}{(4m-3)} = -\dfrac{\tau}{1-\tau/2} \\ +\dfrac{2}{(4m-1)} = +\dfrac{\tau}{1+\tau/2} \end{cases}, \qquad \tau = \tau(m) = \frac{1}{(2m-1)} > 0.$$

The use of the new variable defines the functions $x_m = x(\tau)$ and $y_m = y(\tau)$ in such a way that $x(\tau) = y(-\tau)$, i.e., *both* of them are given by the *same* series in τ,

$$z = \begin{Bmatrix} x_m \\ y_m \end{Bmatrix} = \frac{\mu^2}{\pi^2}\tau^2 \pm \frac{\mu^2}{\pi^2}\tau^3 + \left(\frac{3\mu^2}{4\pi^2} + \frac{\mu^4}{\pi^4}\right)\tau^4 \pm \left(\frac{\mu^2}{2\pi^2} - 2\frac{\mu^4}{\pi^5} + 2\frac{\mu^4}{\pi^4}\right)\tau^5 + \cdots.$$

As expected, $x(\tau)$ grows more rapidly with τ so that we arrived at an independent, non-trigonometric proof that $x_m > y_m$ for all m for which these series converge. Unfortunately, in contrast to our previous formula (25) which offers a systematic improvement of convergence with respect to *both* the increasing couplings $\mu = \xi/2$ *and* the decreasing excitations $m \ll \infty$, the latter two power series in τ have an error term $\mathcal{O}(\mu^2)$ so that they remain less useful unless the coupling μ remains very small.

4.2. Matrix elements and wavefunctions

As long as we work just with the four-dimensional matrix problem (11), it makes sense to derive the perturbed wavefunctions directly from its $a = 1/2$ version with abbreviations $S = \sin(\kappa/2)$ and $C = \cos(\kappa/2)$,

$$\begin{pmatrix} S & 0 & -C & 0 \\ 0 & S & 0 & -S \\ -C & \xi\kappa^{-1}S & S & 0 \\ \xi\kappa^{-1}S & C & 0 & C \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \\ \gamma \\ \delta \end{pmatrix} = 0. \tag{26}$$

An analysis of such a compactified Schrödinger equation must be performed separately in the two or three different domains of κ.

4.2.1. Special cases of the levels when $S = 0$ or $C = 0$. Once we admit that $S = 0$, we infer that $\alpha = \gamma = 0$ and $\beta = -\delta \neq 0$ while $C = \pm 1$. Wavefunctions $\psi(x) \sim \sin\kappa x$ vanish precisely at the points of interaction and so they 'do not see it' and remain independent of ξ. The whole family of these $\psi(x)$ coincides, at all real non-Hermiticites ξ, with the pure square-well states $\psi_4(x)$, $\psi_8(x)$, ... with subscripts $n \equiv 0 \,(\mathrm{mod}\, 4)$.

In another special case of the matrix elements such that $C = 0$, wavefunctions may be re-normalized to having antisymmetric real part,

$$\psi(x) = \begin{cases} \psi_L(x) = \sin\kappa(x+1), & x \in (-1, -1/2) \\ \psi_C(x) = -\mathrm{i}\xi\kappa^{-1}\cos\kappa x - \sin\kappa x, & x \in (-1/2, 1/2) \\ \psi_R(x) = \sin\kappa(x-1), & x \in (1/2, 1). \end{cases} \tag{27}$$

At all ξ the corresponding energies remain also equal to the Hermitian square-well values $E_2, E_6, \ldots$. We may note that there exists also a non-trivial symmetric imaginary part of $\psi(x)$ which vanishes for $|x| > 1/2$ and which grows in proportion to the coupling ξ.

4.2.2. Generic Schrödinger equation. At the generic matrix elements $S \neq 0 \neq C$ our four-dimensional Schrödinger equation (26) implies the simplification $\delta = \beta$. This may be inserted in our ansatz (9) for wavefunctions and enables us to drop the second line in equation (26) as redundant,

$$\begin{pmatrix} S & 0 & -C \\ -C & \xi\kappa^{-1}S & S \\ \xi\kappa^{-1}S & 2C & 0 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix} = 0. \tag{28}$$

This simplifies the derivation of the other two closed formulae,

$$\beta = \delta = -\frac{\xi}{2\kappa}\tan(\kappa/2)\alpha, \qquad \gamma = \tan(\kappa/2)\alpha. \tag{29}$$

We are left with a single equation requiring that the secular determinant vanishes. We may freely choose a normalization $\alpha = 1$ and conclude that the determination of the wavefunctions is completed. Their explicit perturbative dependence on the excitation number m is mediated by formulae (21) and (25).

5. The coupling dependence of the solutions

Our reduced secular equation (17) contains the trigonometric functions S and C. In the opposite direction we may abbreviate $\varrho = \xi/\kappa$ and eliminate S and C, transforming this secular equation into one of the following two equivalent new formulae,

$$S^2 = \frac{1}{2-\varrho^2/2}, \qquad C^2 = \frac{1-\varrho^2/2}{2-\varrho^2/2}. \tag{30}$$

These relations re-define the matrix elements in our four-dimensional 'perturbed' Schrödinger equation (26) as functions of an alternative new variable ϱ which remains small in the weak-coupling regime.

5.1. An illustration with $z = x_m$

The choice of $z = x_m$ covers the energy levels E_1 (= ground state), E_5, E_9 etc. They are all slightly greater than their 'unperturbed', square-well $\xi = 0$ predecessors.

From our previous analysis of the subset of eigenvalues E_{4m-3} corresponding to $z = x_m$ we infer that below the level crossing, i.e., for all not too large couplings $\xi < \xi_{(4m-3)\otimes(4m-2)} = \sqrt{2}\pi(2m-1)$ we may take the square roots in equation (30) unambiguously. Without any loss of generality (i.e., up to an irrelevant overall sign), we shall evaluate our matrix elements in accordance with the unique recipe

$$S = S_x(\varrho) = \sqrt{\frac{1}{2-\varrho^2/2}} > C = C_x(\varrho) = \sqrt{\frac{1-\varrho^2/2}{2-\varrho^2/2}} > 0. \tag{31}$$

In both these functions we may consider the quantity ϱ small and employ their known Taylor expansions,

$$\sqrt{2}S_x(\varrho) = 1 + \frac{1}{8}\varrho^2 + \frac{3}{128}\varrho^4 + \frac{5}{1024}\varrho^6 + \frac{35}{32\,768}\varrho^8 + \frac{63}{262\,144}\varrho^{10} + O(\varrho^{12})$$
$$\sqrt{2}C_x(\varrho) = 1 - \frac{1}{8}\varrho^2 - \frac{5}{128}\varrho^4 - \frac{13}{1024}\varrho^6 - \frac{141}{32\,768}\varrho^8 - \frac{399}{262\,144}\varrho^{10} + O(\varrho^{12}).$$

Another Taylor series carrying a weak-coupling perturbation expansion character,

$$S_x(\varrho)/C_x(\varrho) = 1 + \frac{1}{4}\varrho^2 + \frac{3}{32}\varrho^4 + \frac{5}{128}\varrho^6 + \frac{35}{2048}\varrho^8 + O(\varrho^{10})$$

enters formulae (29) which define all the components $\gamma = \gamma(\varrho) \equiv \delta$ and $\beta = \beta(\varrho)$ of the perturbed wavefunctions.

5.1.1. The second special case with $z = y_m$. The fourth quarter of the set of all eigenvalues comprises the energies E_{4m-1} which lie below their unperturbed partners and which correspond to the choice of $z = y_m$. In this case we have to take the square roots in equation (30) in accordance with this modified expectation,

$$S = S_y(\varrho) = \sqrt{\frac{1}{2-\varrho^2/2}} > -C = -C_y(\varrho) = \sqrt{\frac{1-\varrho^2/2}{2-\varrho^2/2}} > 0. \tag{32}$$

The necessary parallel modification of all the previous $z = x_m$ results and formulae is trivial.

5.2. Wavefunctions in dependence on both ξ and $1/m$

Our wavefunctions have to be represented in terms of both the complementary and independent measures of the non-Hermiticity $\lambda = \lambda(m)$ and $\mu = \xi/2$. The final transition from the intermediate auxiliary quantity ϱ to this original pair of expansion parameters profits from the feasibility of the Taylor-expansion technique. Up to corrections $O(\lambda^9\mu^8)$ we have the following final result for the matrix elements in equation (26):

$$\sqrt{2}S_x[\varrho(\lambda)] \approx 1 + \frac{1}{2}\mu^2\lambda^2 + \frac{3}{8}\mu^4\lambda^4 - \mu^4\lambda^5 + \frac{5}{16}\mu^6\lambda^6 - \frac{5}{2}\mu^6\lambda^7 + \left(\frac{35}{128}\mu^8 - \frac{1}{2}\mu^6\right)\lambda^8,$$

$$\sqrt{2}C_x[\varrho(\lambda)] \approx 1 - \frac{1}{2}\mu^2\lambda^2 - \frac{5}{8}\mu^4\lambda^4 + \mu^4\lambda^5 - \frac{13}{16}\mu^6\lambda^6 + \frac{7}{2}\mu^6\lambda^7 + \left(-\frac{141}{128}\mu^8 + \frac{1}{2}\mu^6\right)\lambda^8.$$

This converts our Schrödinger equation (26) of the form $Q(\lambda, \mu)\vec{\psi} = 0$ into its power-series four-by-four matrix version

$$[Q(0,0) + \mu^2\lambda^2 Q_{[1]} + \mu^4\lambda^4 Q_{[2]} + \mu^4\lambda^5 Q_{[3]} + \cdots]\vec{\psi}(\lambda, \mu) = 0.$$

The standard Rayleigh–Schrödinger perturbation theory [1] might apply and define the sequence of corrections, order-by-order in both our small parameters. The exact solvability of our problem facilitates the underlying manipulations and reduces the abstract algorithm to the explicit formulae (29) where the only ingredient we need to know is the expansion of the single auxiliary factor S/C. It is easy to derive its sixth-order weak-coupling form

$$\tan\left[\kappa_m\left(\tfrac{1}{2}, 2\mu\right)\right] \approx 1 + \mu^2\lambda^2 + \tfrac{3}{2}\mu^4\lambda^4 - 2\mu^4\lambda^5 + \tfrac{5}{2}\mu^6\lambda^6 - 8\mu^6\lambda^7 + \left(\tfrac{35}{8}\mu^8 - \mu^6\right)\lambda^8$$

as well as all its further higher order improvements whenever needed.

6. Summary and outlook

We described an application of the PTSQM formalism to a toy-model Hamiltonian H with the real energies $E_n = \kappa_n^2$ which remain non-degenerate for $\xi < \xi_{1\otimes 2}$. The set of bound states $|n\rangle$ (9) is not orthogonal since $H^\dagger = \mathcal{P}H\mathcal{P} \neq H$. Still, in our Hilbert space we may construct a biorthogonal basis using the second set of eigenstates of $H^\dagger$ corresponding to the same spectrum of course. They will be distinguished by the double-bra/ket symbols (e.g., $\langle\langle n|$ or $|n\rangle\rangle$, respectively), being most naturally understood as the 'left eigenstates of H' [25] defined by equation

$$H^\dagger|m\rangle\rangle = E_m|m\rangle\rangle = \mathcal{P}H\mathcal{P}|m\rangle\rangle.$$

Due to the involutivity of the parity ($\mathcal{P}^2 = I$) and due to the non-degeneracy of the spectrum we know that $\mathcal{P}|m\rangle\rangle$ must be proportional to $|m\rangle$ so that we are free to define

$$|m\rangle\rangle = q_m^*\mathcal{P}|m\rangle$$

using any normalization constant q_m^* (for our future convenience we write here the star * which denotes complex conjugation). It is also easy to deduce the law of biorthogonality $\langle\langle n|m\rangle \sim \delta_{mn}$ (hint: subtract the two suitably pre-multiplied equations $H|m\rangle - E_m|m\rangle$ and $\langle\langle n|H = E_n\langle\langle n|$). Once we evaluate all the overlaps $R_n = \langle\langle n|n\rangle$, we may formally write down the explicit decomposition of the unit operator,

$$I = \sum_{n=1}^{\infty} |n\rangle \frac{1}{R_n} \langle\langle n| = \sum_{n=1}^{\infty} |n\rangle\rangle \frac{1}{R_n^*} \langle n|$$

as well as the spectral decompositions of our two forms of the Hamiltonian,

$$H = \sum_{n=1}^{\infty} |n\rangle \frac{E_n}{R_n} \langle\langle n|, \qquad H^\dagger = \sum_{n=1}^{\infty} |n\rangle\rangle \frac{E_n}{R_n^*} \langle n|. \tag{33}$$

In practice, we determine the values of R_n by calculating matrix elements of parity which *are* all real but which *cannot* be all of the same sign, $\langle n|\mathcal{P}|n\rangle = R_n/q_n$.

The key step now lies in making the PTSQM formalism compatible with the postulates of quantum theory by an introduction of some new operator η of 'the physical' metric in Hilbert space. We remind the reader that it need not be involutive ($\eta^2 \neq I$ in general [5]) but it must be Hermitian and positive definite, i.e., $\eta = \eta^\dagger \neq \mathcal{P}$ (in this sense, the indeterminate $\mathcal{P}$ is *not* a metric). The main purpose of the search for such a metric η is that it makes our Hamiltonian quasi-Hermitian and, hence, physical,

$$H^\dagger = \eta H \eta^{-1}.$$

Let us now re-interpret this relation as an equation for η which we have to solve. In the light of equation (33) we have

$$\sum_{n=1}^{\infty} \eta|n\rangle \frac{E_n}{R_n} \langle\langle n| = \sum_{m=1}^{\infty} |m\rangle\rangle \frac{E_m}{R_m^*} \langle m|\eta \tag{34}$$

which implies that, in general,

$$\eta = \sum_{m,n=1}^{\infty} |n\rangle\rangle M_{nm} \langle\langle m|.$$

The backward insertion of such an ansatz in equation (34) gives, at all n and m, the condition $E_n M_{nm} = M_{nm} E_m$ with the solution $M_{nm} = c_n \delta_{nm}$. The Hermiticity and positivity constraints restrict finally the freedom of the choice of the optional sequence of c_n to the real and positive parameters $c_n \equiv \eta_n > 0$. Vice versa, *any* choice $\eta_n^{(toy)}$ of the latter sequence defines an eligible operator of the metric,

$$\eta_{(\mathrm{toy})} = \sum_{n=1}^{\infty} |n\rangle\rangle \eta_n^{(\mathrm{toy})} \langle\langle n| = \eta_{(\mathrm{toy})}^\dagger > 0. \tag{35}$$

We arrive at a climax and summary of our present message. At any coupling in the allowed range $\xi < \xi_{1\otimes 2} \approx 4.44$ the eigenstates $|n\rangle = |n, \xi\rangle$ and $|n\rangle\rangle = |n, \xi\rangle\rangle$ pertaining to our toy model $H = H(\xi)$ have been shown to exhibit an asymptotic suppression of all the influence of their non-Hermiticity at all sufficiently large excitations,

$$|n, \xi\rangle\rangle \approx |n, 0\rangle\rangle, \qquad |n, \xi\rangle \approx |n, 0\rangle, \qquad n > N = N(\xi). \tag{36}$$

The value of the cut-off $N(\xi)$ has been shown to grow quite slowly both with the non-Hermiticity ξ and with the required precision of the approximation (36). We may conclude that on an optional level of precision (and assuming that we choose $\eta_n^{(\mathrm{toy})} = 1$ in equation (35)

for all $n > N(\xi)$) we may always treat any pertaining metric $\eta_{(\mathrm{toy})}$ as an operator which differs from the unit operator just by a finite dimensional, N-parametric separable modification,

$$\eta_{(\mathrm{toy})} \approx I - \sum_{n=1}^{N(\xi)} |n,0\rangle\rangle\langle\langle n,0| + \sum_{n=1}^{N(\xi)} |n,\xi\rangle\rangle \eta_n^{(\mathrm{toy})} \langle\langle n,\xi|. \tag{37}$$

This is the property which our toy model shares with the other non-Hermitian square-well models as available and studied in the recent literature [15–17, 30]. Still, as a rule, the majority of properties of the latter models looks *much* less accessible to any non-numerical treatment. In contrast to that, the present energies as well as wavefunctions preserve a compact and closed form, particularly transparent in the most symmetric case with $a = 1/2$. For illustrative purposes this enabled us to construct, entirely systematically and in a fully non-numerical manner, an explicit sample of the order-by-order corrections in approximations (36). Thus, our model as well as formulae may be expected to find an immediate application in the key separable formula (37) which acquires, in this manner, the form of an explicit perturbation-series recipe which may be systematically improved up to (in principle, arbitrary) precision.

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